Emergence of rotational bands from ab initio nuclear structure calculations

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SciDAC project – NUCLEI
lead PI: Joe Carlson (LANL)
http://computingnuclei.org

PetaApps award
lead PI: Jerry Draayer (LSU)

INCITE award – Computational Nuclear Structure
lead PI: James P Vary (ISU)

NERSC

Ab initio nuclear physics – Quantum many-body problem

- Given a Hamiltonian operator

$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

  solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1, \ldots, r_A) = \lambda\,\Psi(r_1, \ldots, r_A)$$

  - eigenvalues λ discrete (quantized) energy levels
  - eigenvectors: $|\Psi(r_1, \ldots, r_A)|^2$ probability density for finding nucleons 1, …, A at r_1, …, r_A
- Self-bound quantum many-body problem, with $3(A-1)$ degrees of freedom
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Strong interactions, with both short-range and long-range pieces

No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core Configuration Interaction
  - all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional
- In practice
  - truncate basis
  - study behavior of observables as function of truncation
- Computational challenge
  - construct large $(10^{10} \times 10^{10})$ sparse symmetric real matrix H_{ij}
  - use Lanczos algorithm to obtain lowest eigenvalues & -vectors

Basis expansion $\Psi(r_1,\ldots,r_A)=\sum a_i\Phi_i(r_1,\ldots,r_A)$

- Many-Body basis states $\Phi_i(r_1,\ldots,r_A)$ Slater Determinants
- Single-Particle basis states $\phi_{ik}(r_k)$ quantum numbers n, l, s, j, m
- Radial wavefunctions: Harmonic Oscillator, Wood–Saxon, Coulomb–Sturmian, Berggren (for resonant states)
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

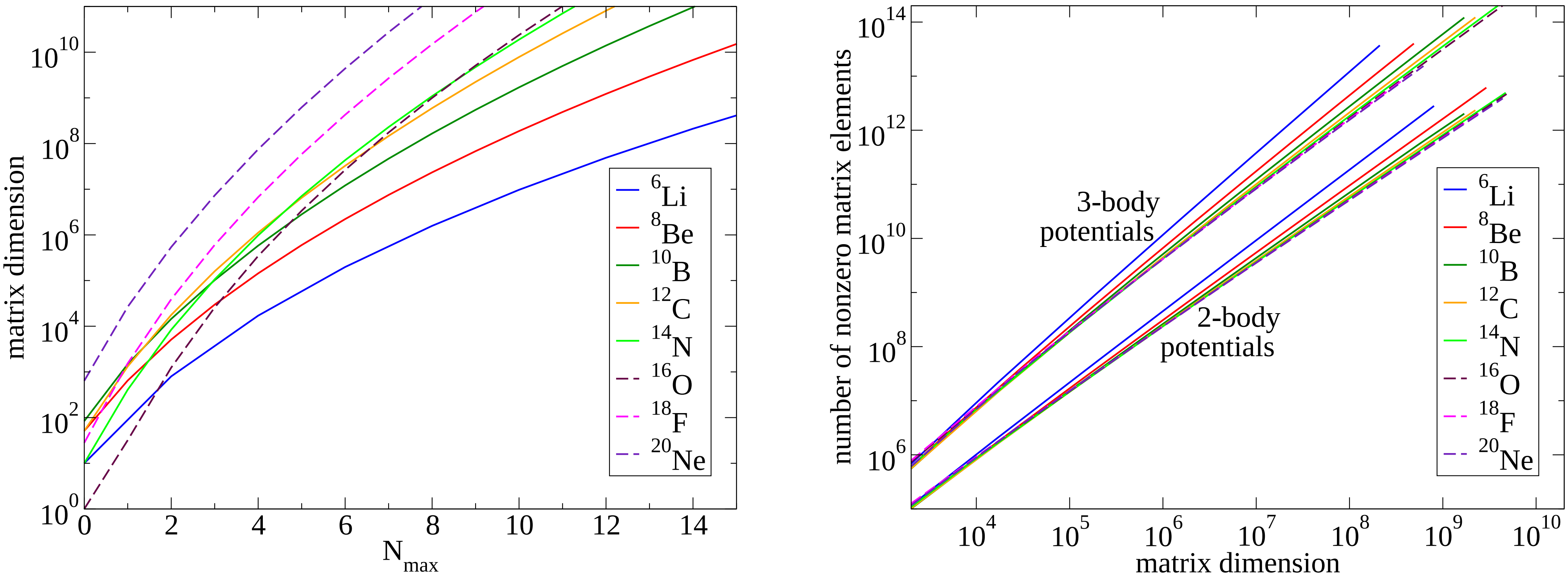
$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle = M|\Phi_i\rangle = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

- N_{max} truncation: Many-Body basis states satisfy

$$\sum_{k=1}^{A}\left(2\,n_{ik}+l_{ik}\right) \le N_0+N_{\text{max}}$$

- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - SU(3) Truncation — Dytrych *et al*, PRL111, 252501 (2013)

NCCI calculations – main challenge



- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$
    for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14} (Edison, Mira, Titan)

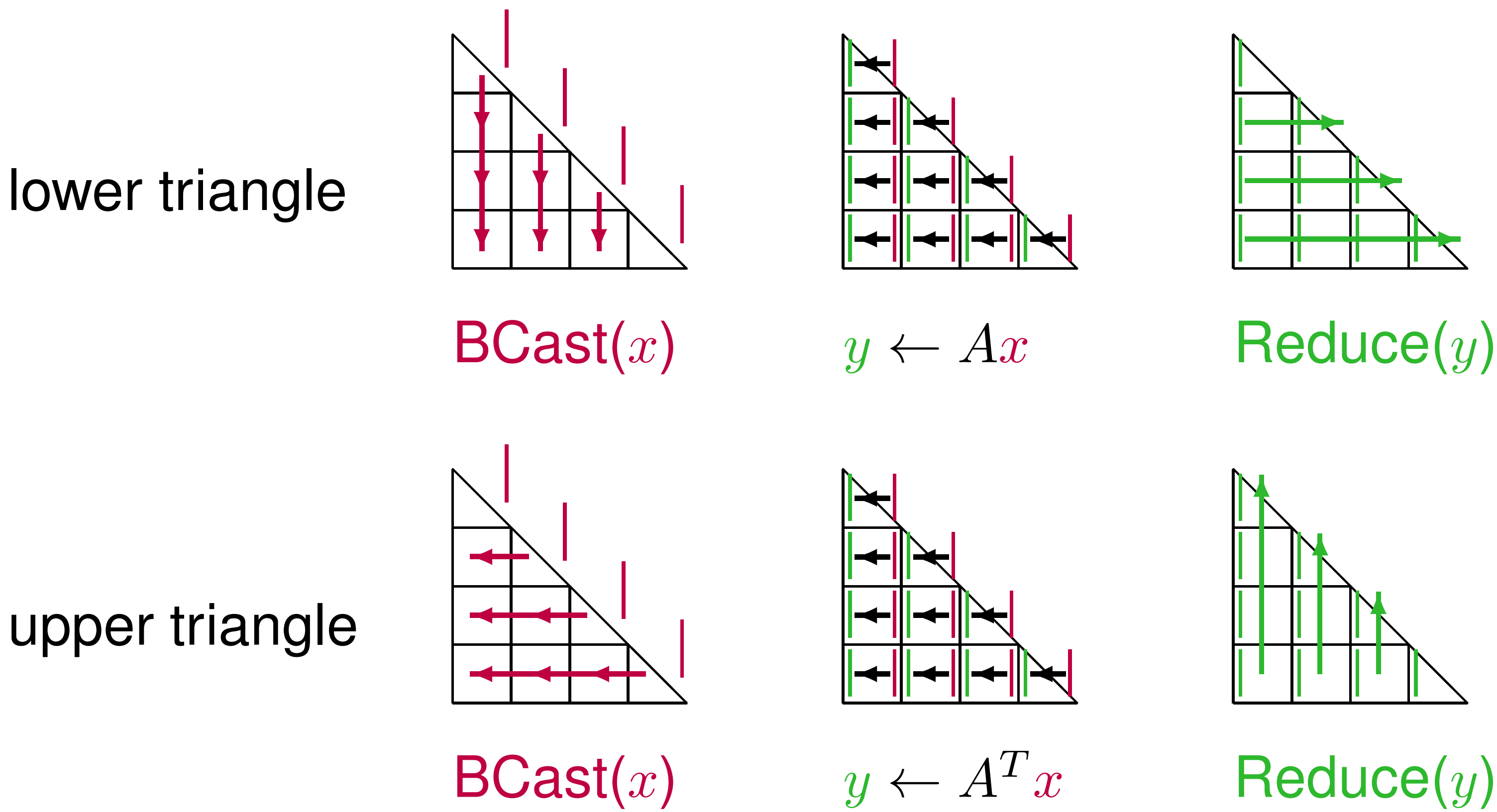
Many Fermion Dynamics – nuclear physics

Configuration Interaction code for nuclear structure calculations

- Platform-independent, hybrid OpenMP/MPI, Fortran 90
- Generate many-body basis space
  subject to user-defined single-particle and many-body truncation
- Construct of many-body matrix H_{ij}
  - determine which matrix elements can be nonzero
    based on quantum numbers of underlying single-particle states
  - evaluate and store nonzero matrix elements
    in compressed row/column format
- Obtain lowest eigenpairs using Lanczos algorithm
  - typical use: 10 to 20 lowest eigenvalues and eigenvectors
  - typically need $\sim$ 400 to $\sim$ 800 Lanczos iterations
  - some applications need hundreds of eigenvalues
- Write eigenvectors (wavefunctions) to disk
- Calculate selected set of observables

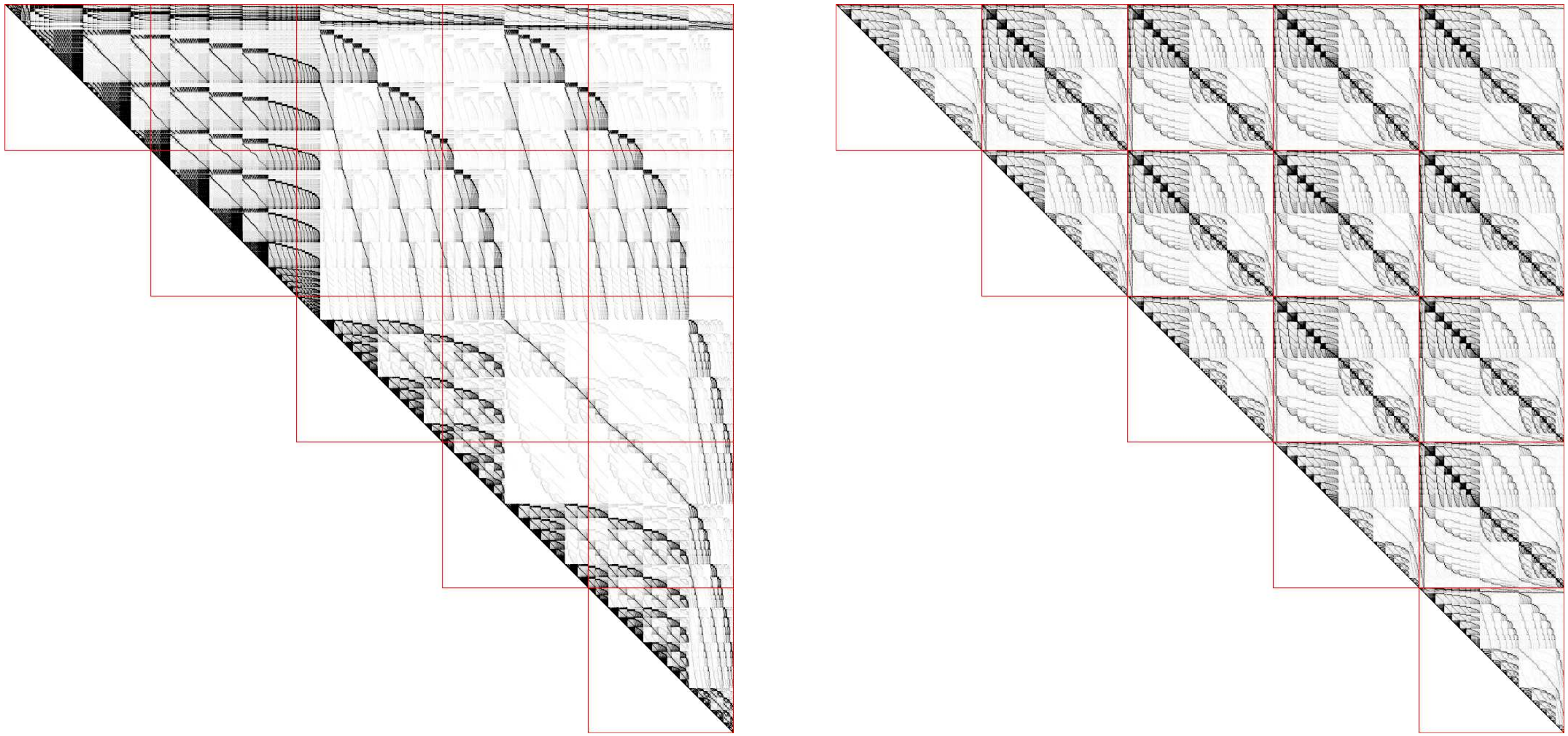
MFDn – 2-dimensional distribution of matrix

- Real symmetric matrix: store only lower (or upper) triangle distributed over $n = d \cdot (d+1)/2$ processors with d “diagonal” proc’s
- In principle, we can deal with arbitrary large dimensions even if we cannot store an entire vector on a single processor
- Communication pattern matrix-vector multiplication



Load balancing

Round-robin distribution of (groups of) many-body basis states

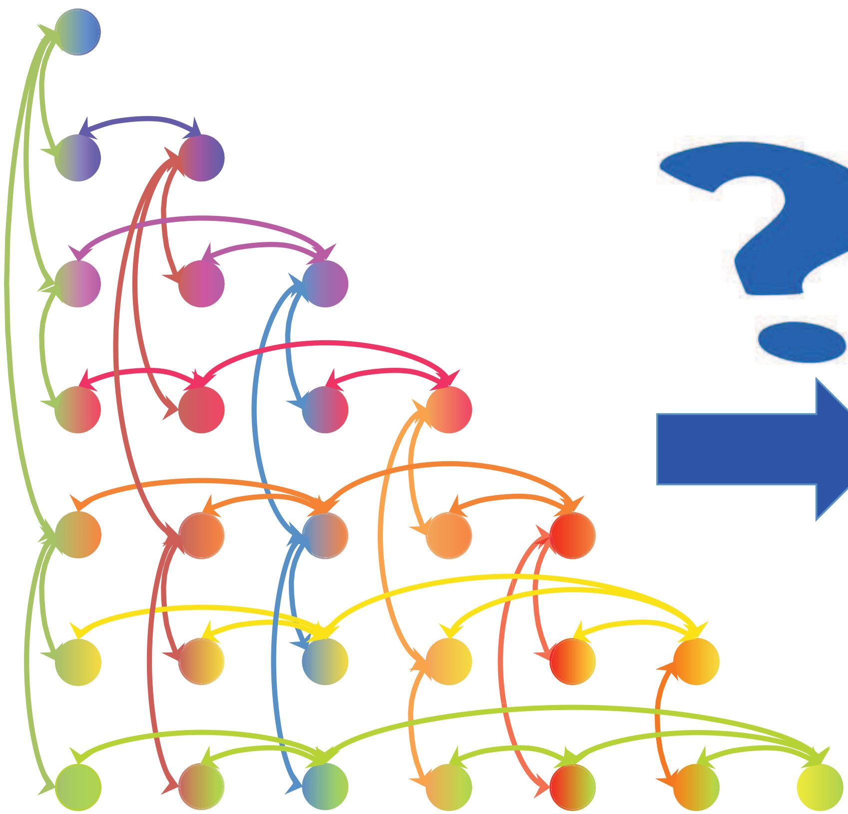


- ^{8}Be at $N_{\max} = 4$ with 3NF on 15 MPI processors
- Dimension 143,792, # nonzero matrix elements 402,513,272

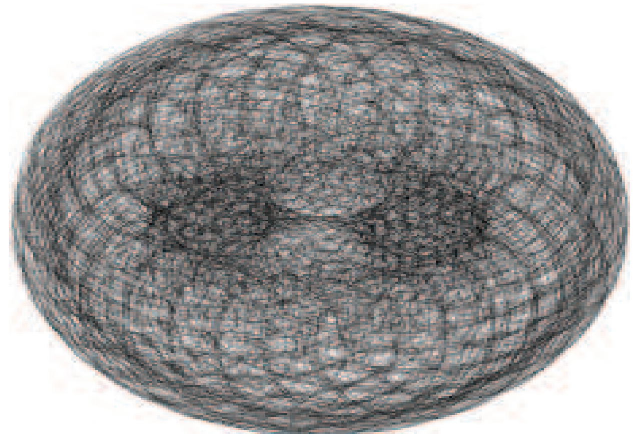
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)

Topology-aware Mapping

MFDn's communication graph

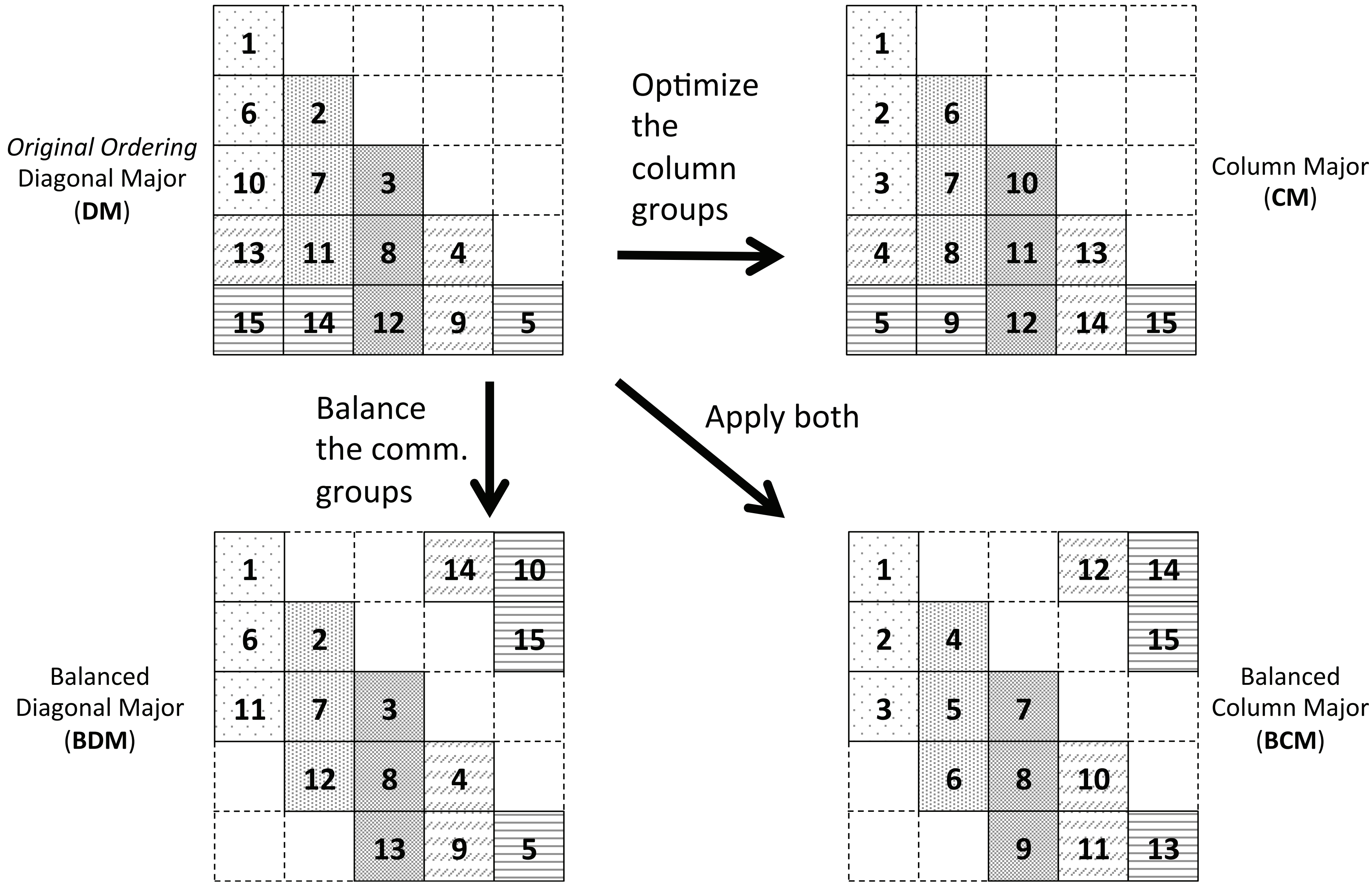


Hopper's 3D Torus



Slide courtesy of Metin Aktulga, LBNL, 2012 (now at MSU)

Different Orderings



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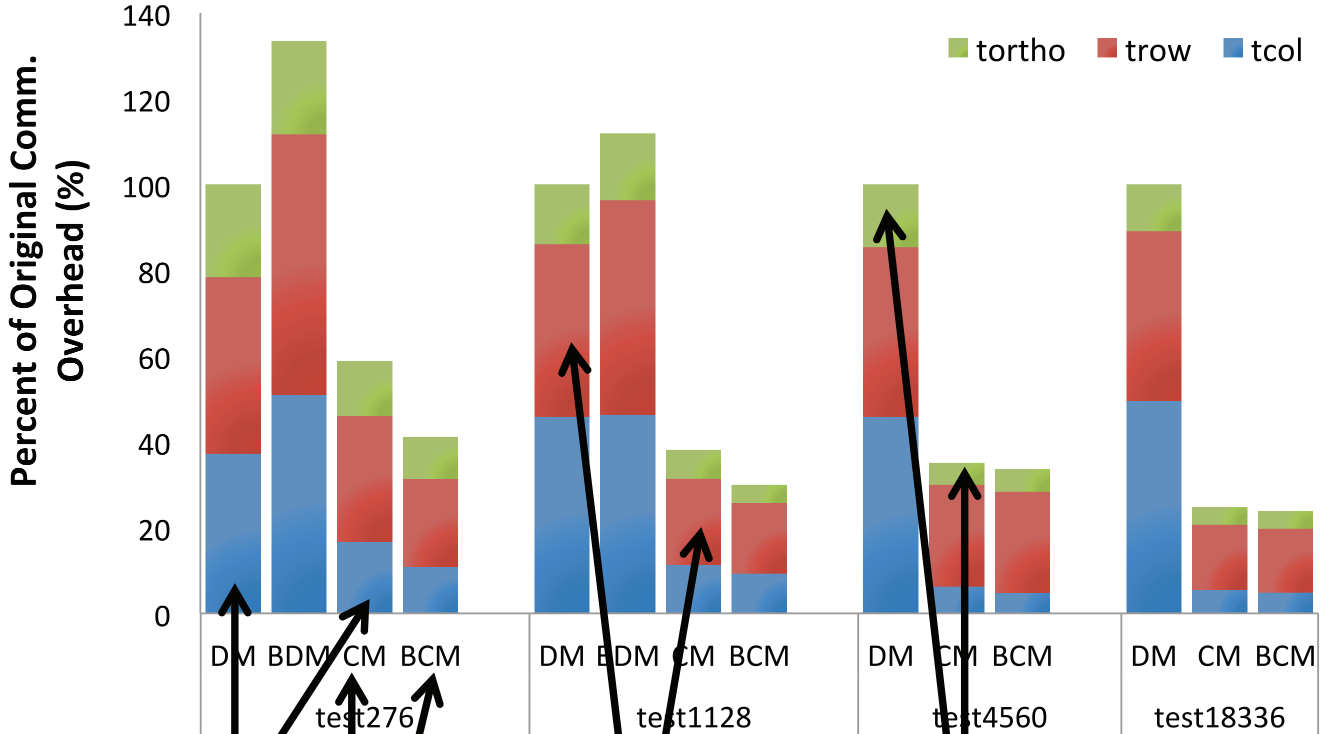
Communication Improvement



significant reductions in column comm overheads

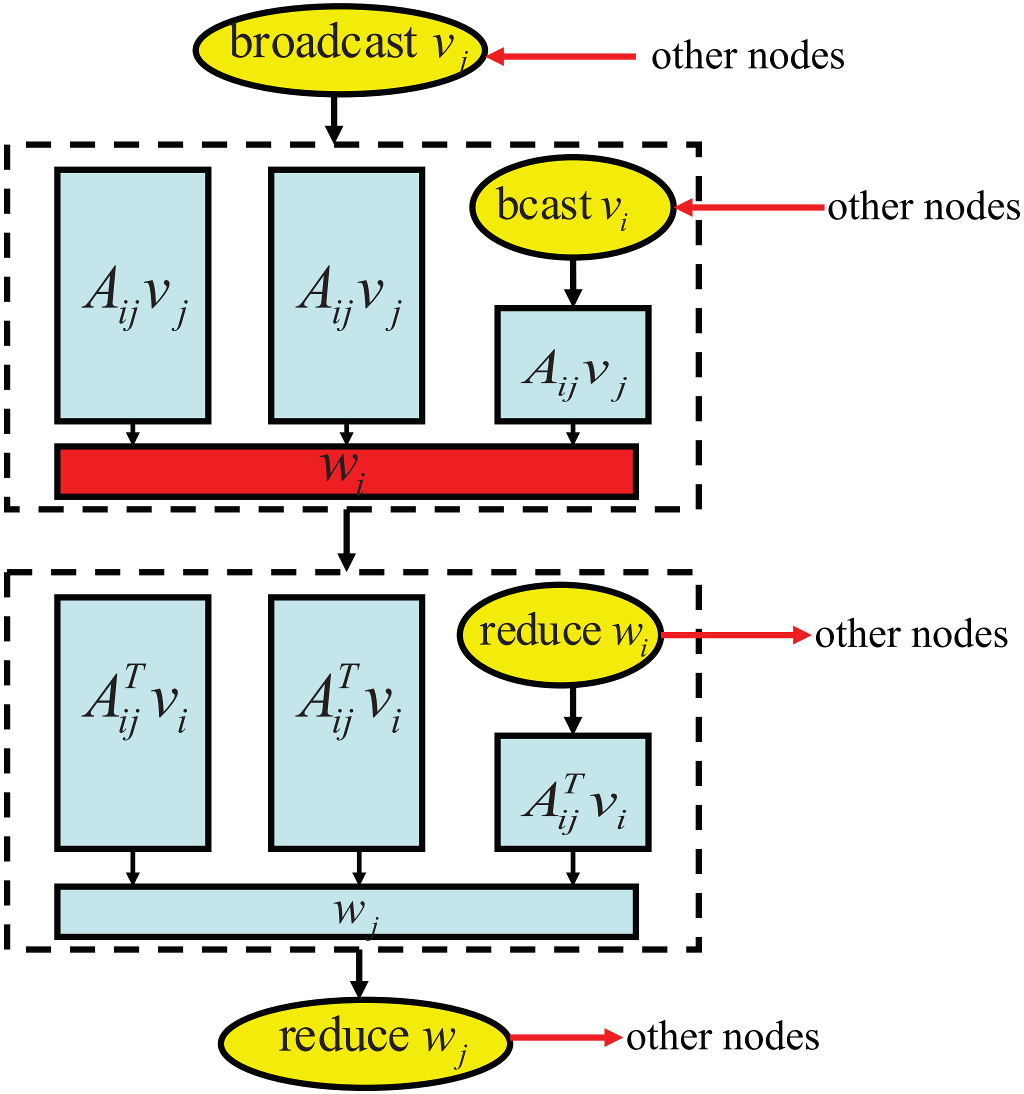
Balancing comm groups pays off

reduced row comm times

ortho. comm time < others as expected

Slide courtesy of Metin Aktulga, LBNL, 2012 (now at MSU)

Communication Hiding: Main Idea



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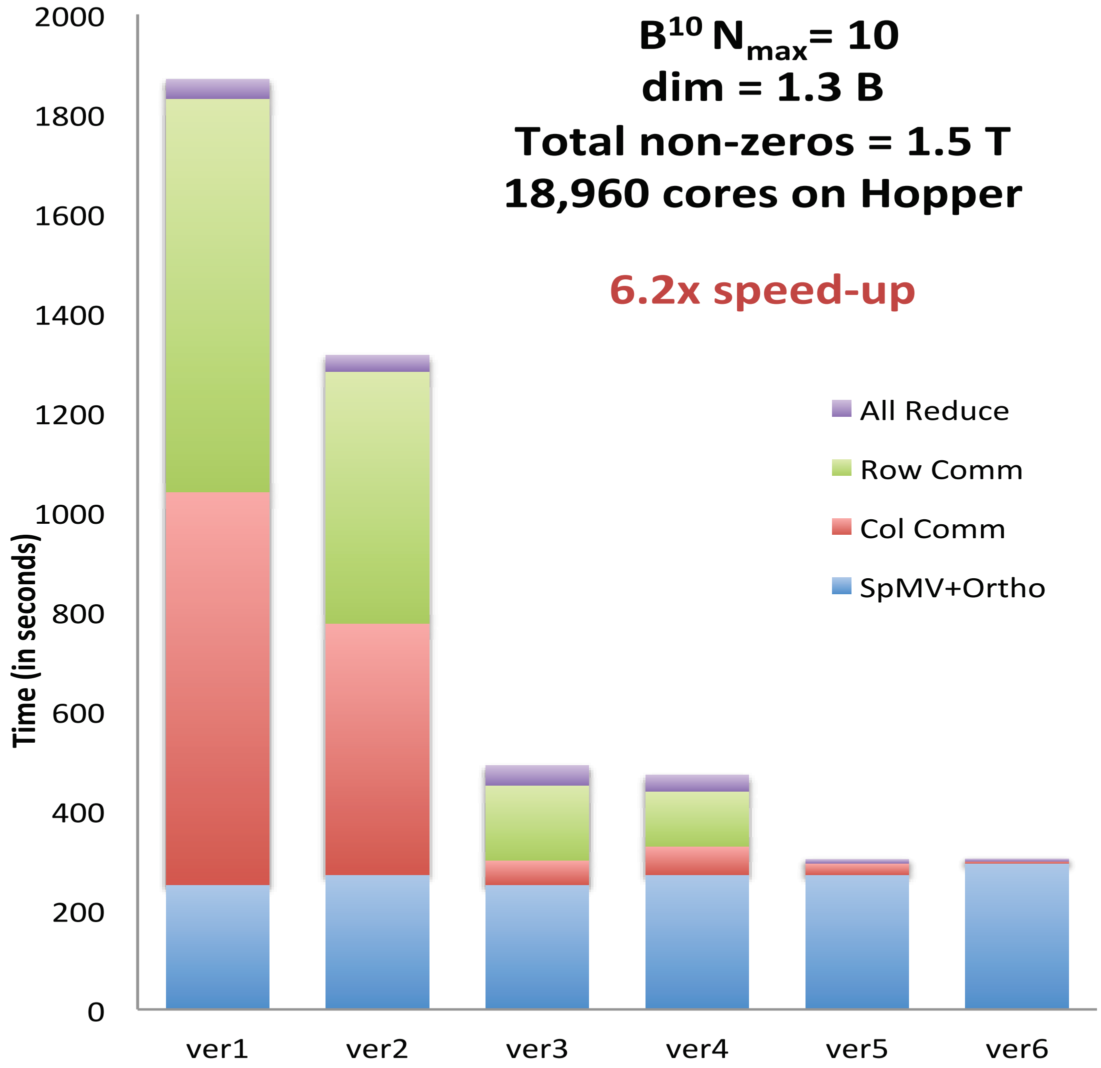
Performance Results



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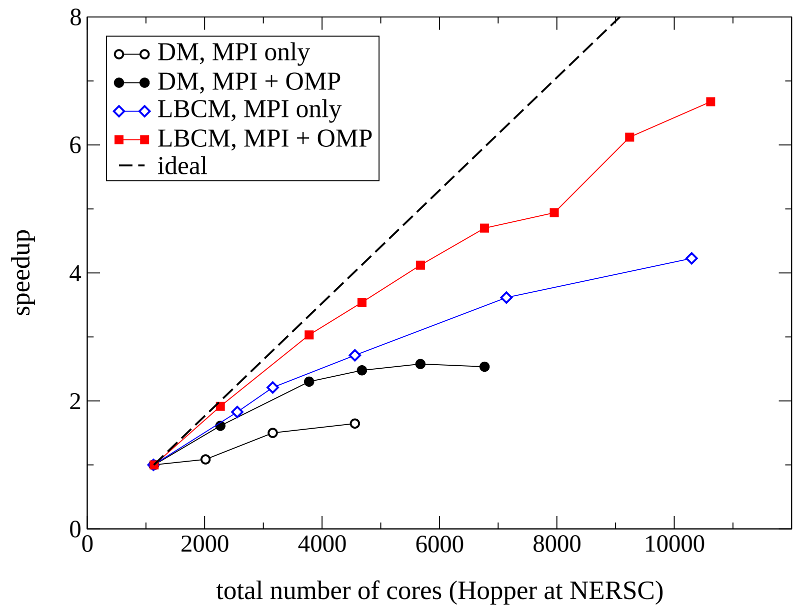
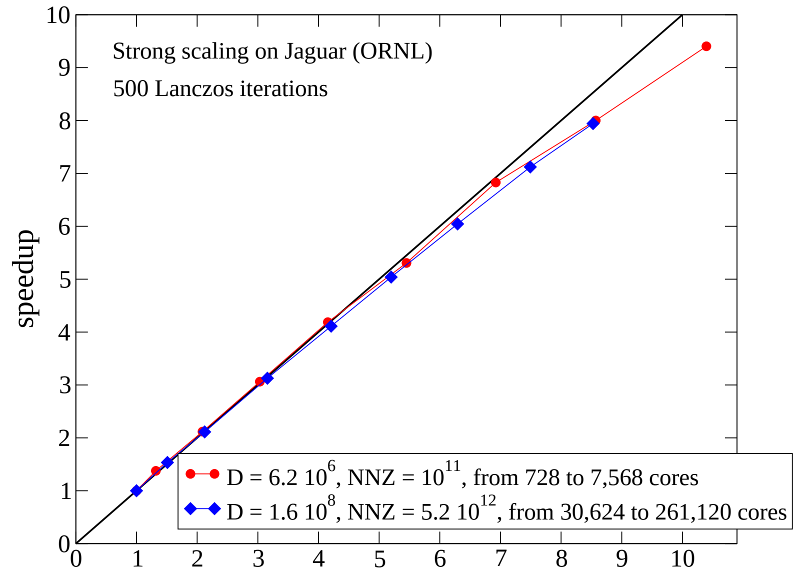
Strong Scaling of MFDn

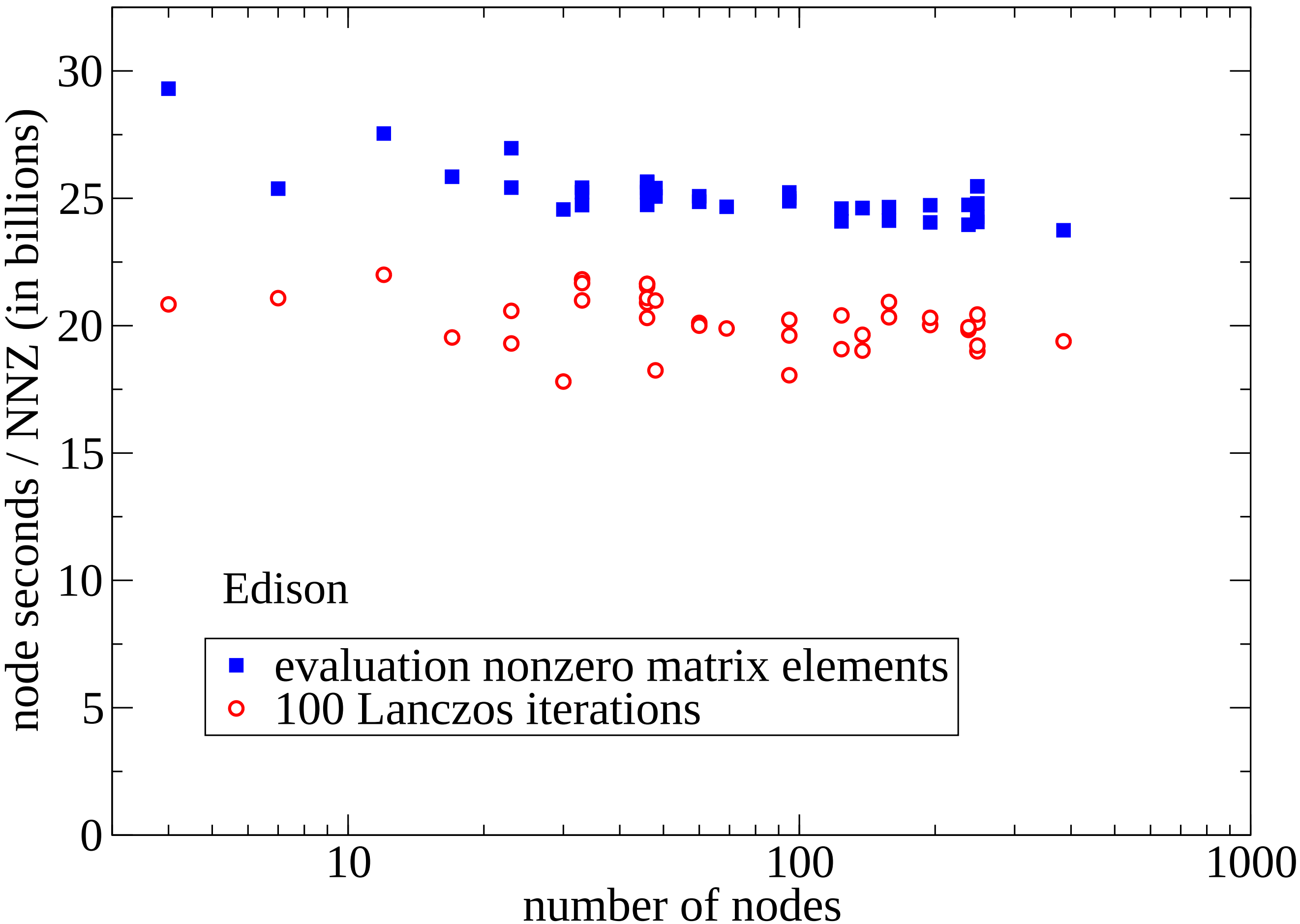
Aktulga, Yang, Ng, Maris, Vary, Concurrency Computat.: Pract. Exper. (2013)





- Understand communication overheads in terms of heuristic network model based on set of compute nodes, physical links between compute nodes, and link capacity
- Hybrid OpenMP/MPI with 1 MPI processor per NUMA node performs better than MPI-only for more than few hundred cores
- Runs with 3-body forces scale better than NN-only runs

Weak Scaling of MFDn



Edison at NERSC: Cray XC30

- two 2.4 GHz Intel 'Ivy Bridge' processors / node
- 12-core/processor (24 cores/node)
- 32 GB/processor (64 GB/node, 2.67 GB/core)
- Cray Aries interconnect (with Dragonfly topology)

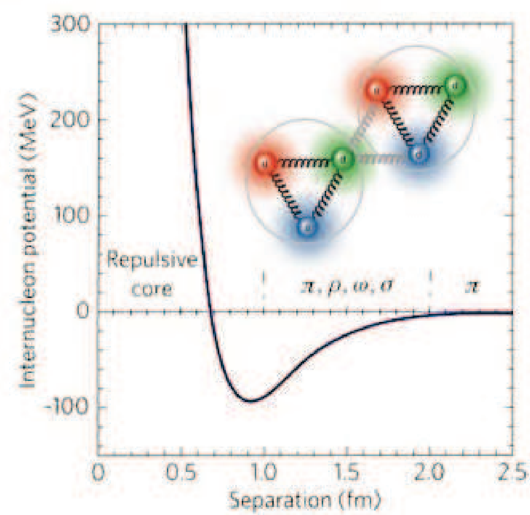
- $A = 10$ NN + 3NF calculations in different basis spaces
- Hybrid OpenMP/MPI
  4 MPI ranks per node, 6 OMP threads / rank

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

$$\hat{\mathbf{H}} \quad = \quad \hat{\mathbf{T}}_{\mathsf{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- ...
- JISP16
- ...

Phenomeological NN interaction: JISP16

JISP16 tuned up to ^{16}O

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

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Realistic nuclear Hamiltonian: Ab exitu approach

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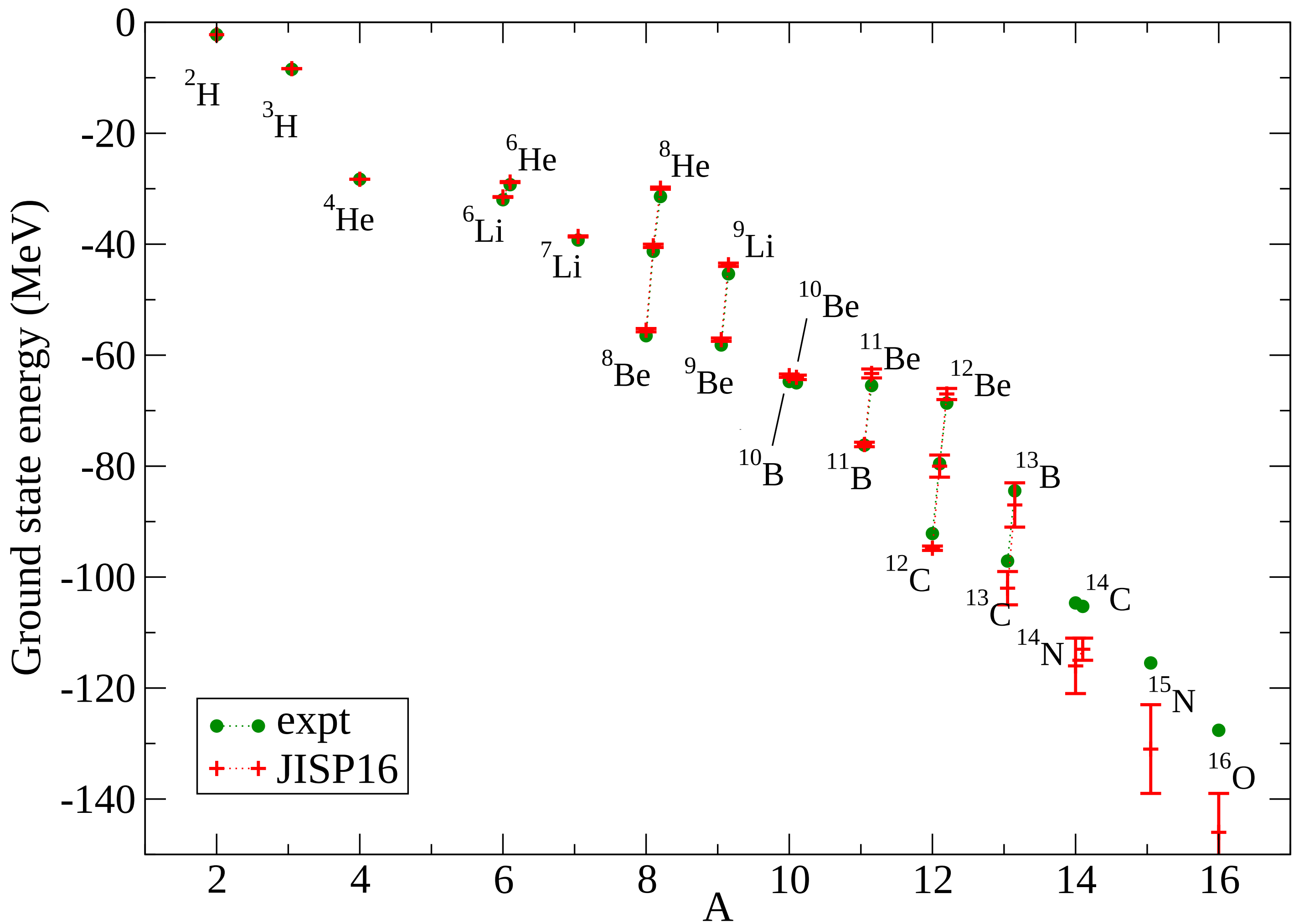
Ground state energy of p-shell nuclei with JISP16

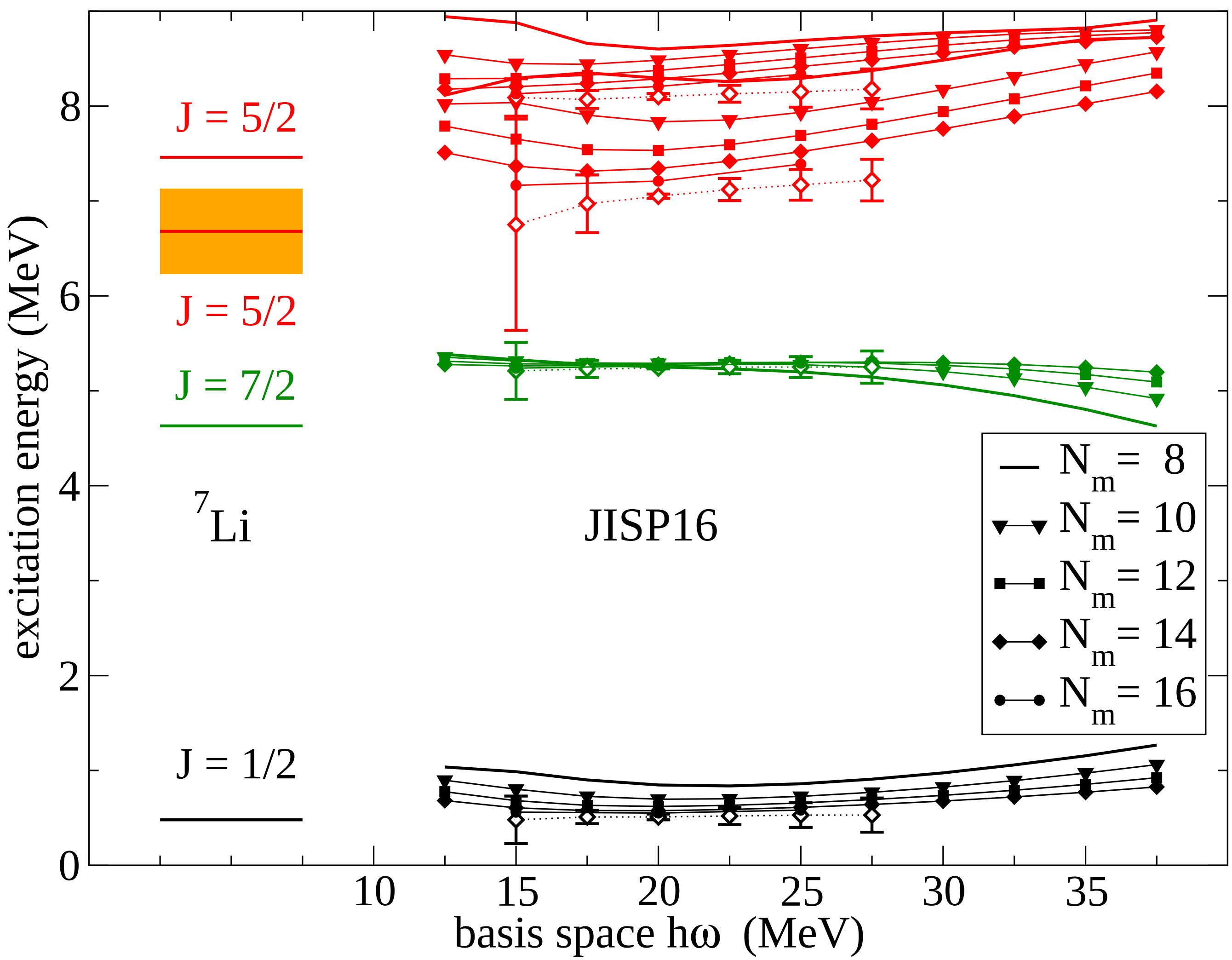
Maris, Vary, IJMPE22, 1330016 (2013)



- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$ MeV) with JISP16

Excitation spectrum 7Li

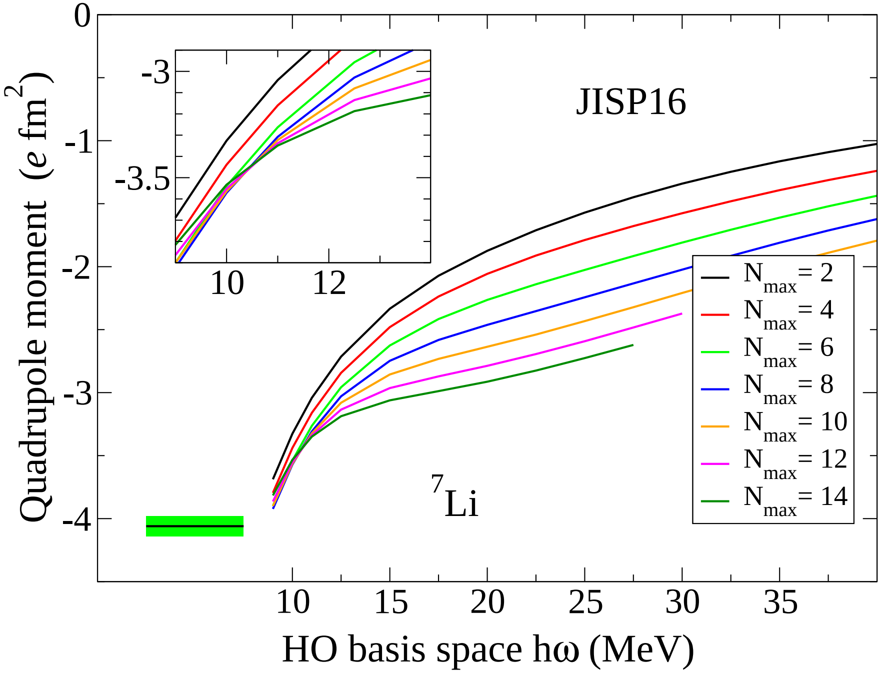
Cockrell, Maris, Vary, PRC86 034325 (2012)

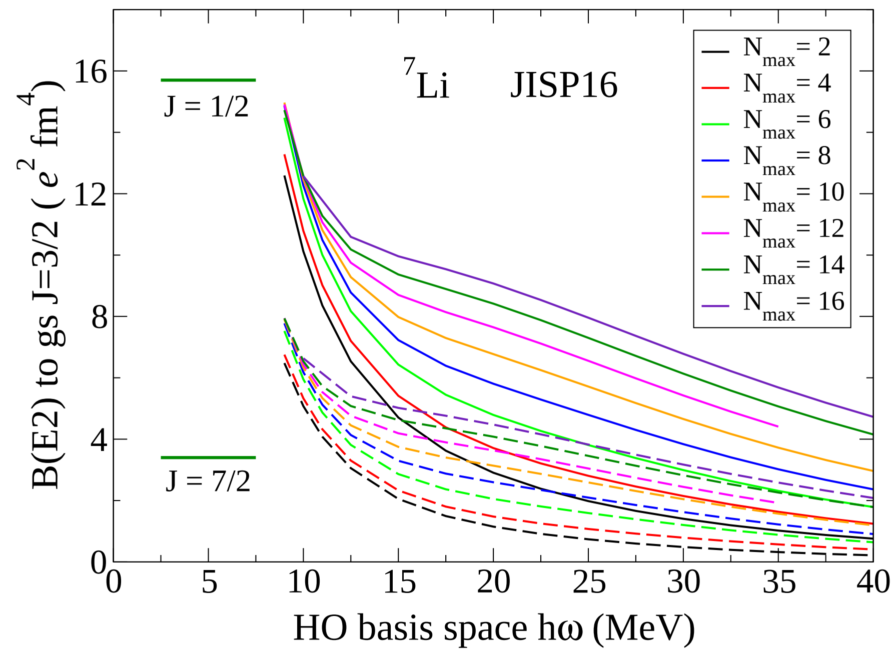


- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum?

Quadrupole moment and B(E2) transition strengths 7Li

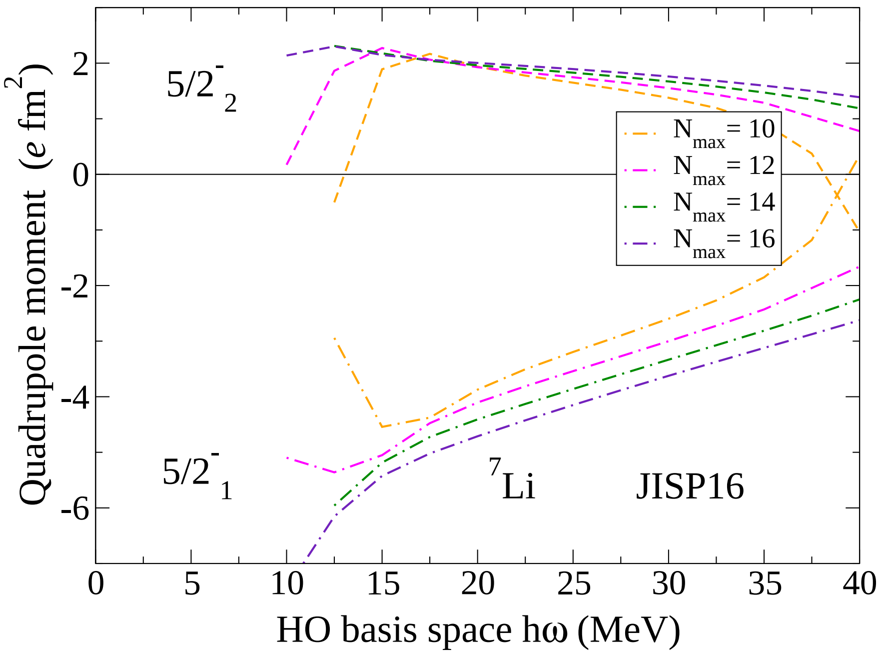
Cockrell, Maris, Vary, PRC86 034325 (2012)

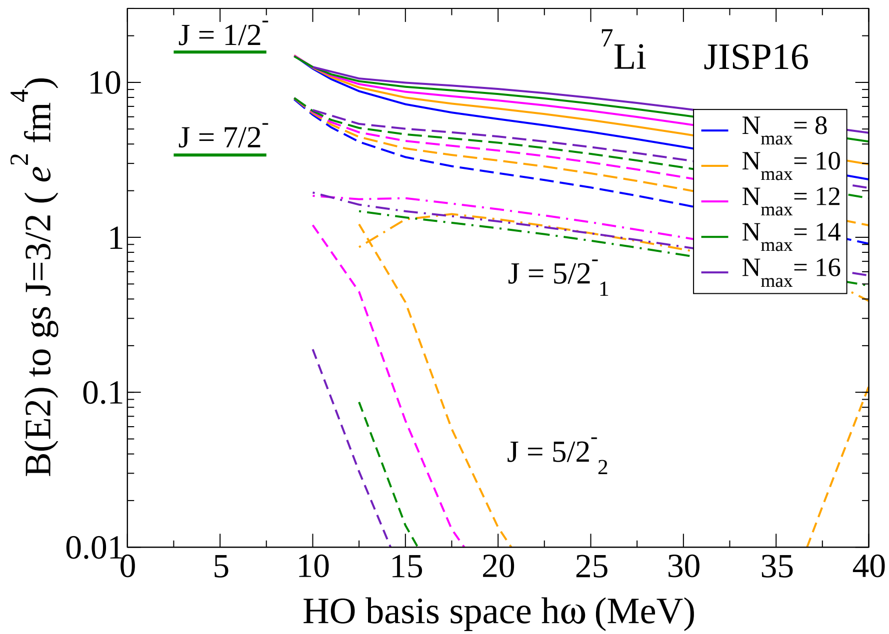




- E2 observables not converged,
  due to gaussian fall-off of HO wavefunction
- Nevertheless, qualitative agreement of $\mathcal{Q}$ and B(E2) with data

Quadrupole moments and B(E2) transitions for $J^\pi = \frac{5}{2}^-$ states

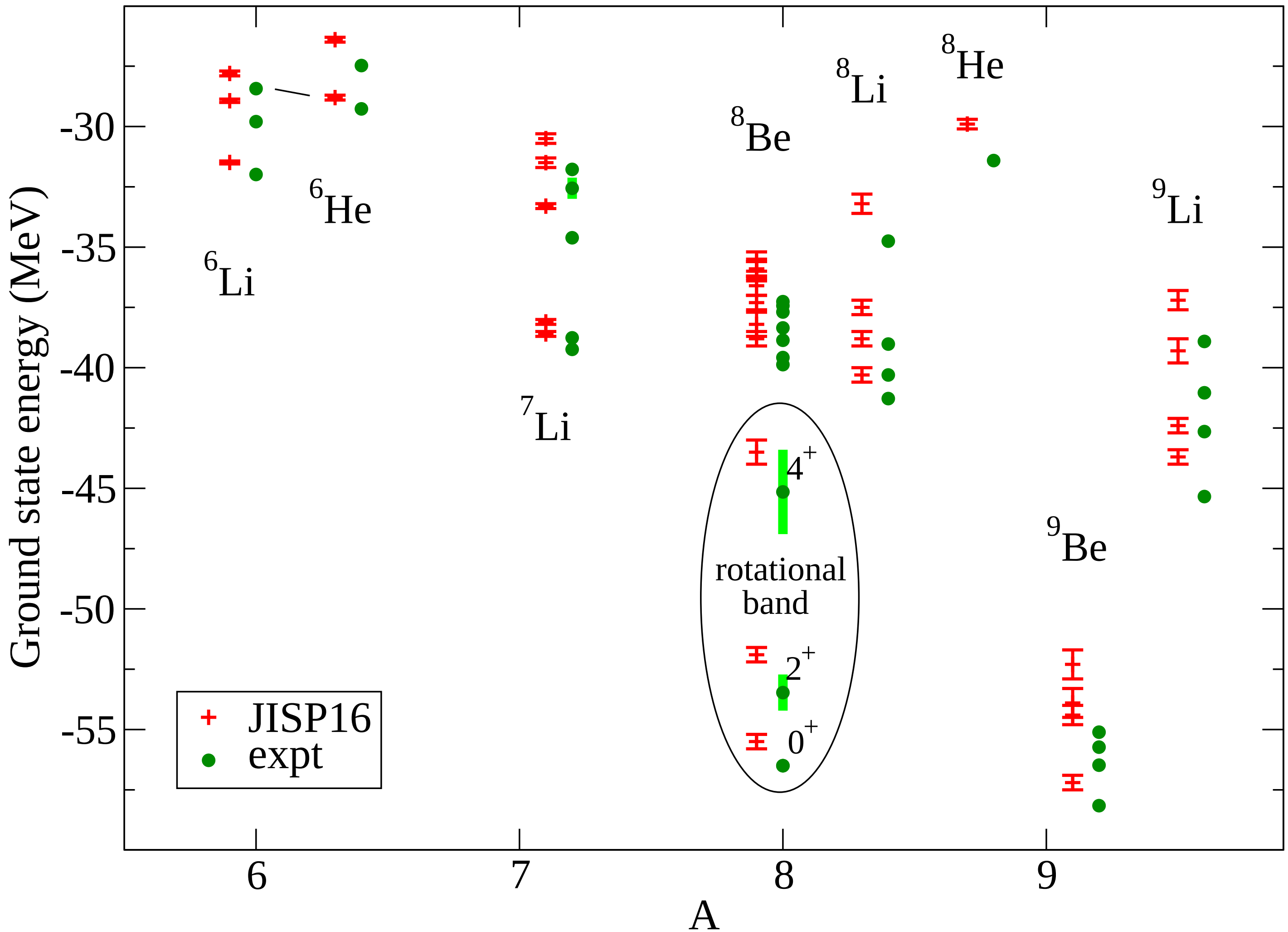




- E2 observables not converged, but nevertheless
  - $J^\pi = \left(\frac{5}{2}^-\right)_1$ large negative quadrupole moment
  - $\frac{1}{2}^-$, $\frac{7}{2}^-$, and $\left(\frac{5}{2}^-\right)_1$ relatively strong B(E2) to g.s.
  - $J^\pi = \left(\frac{5}{2}^-\right)_2$ small positive quadrupole moment, $Q \sim 2\ e$ fm^2, and very small B(E2) to g.s.

Energies of narrow A=6 to A=9 states with JISP16

Maris, Vary, IJMPE22, 1330016 (2013)



- Excitation spectrum narrow states in good agreement with data

Intermezzo: Rotational states

Assuming adiabatic separation of rotational and internal degrees of freedom, a rotational nuclear state $|\psi_{JKM}\rangle$ can be described in terms of an intrinsic state $|\phi_K\rangle$ in a non-inertial frame, combined with the rotational motion of this non-inertial frame

$$|\psi_{JKM}\rangle = \mathcal{N}_{JK} \int d\vartheta \left[\mathscr{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K} \mathscr{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle \right]$$

- Rotational energy

$$E(J) = E_0 + \frac{\hbar^2}{2\mathcal{I}} \left(J(J+1)\right)$$

for $K = \frac{1}{2}$ bands staggering due to Coriolis term

$$E(J) = E_0 + \frac{\hbar^2}{2\mathcal{I}} \left(J(J+1) + a\,(-1)^{J+\frac{1}{2}} \left(J + \tfrac{1}{2}\right) \right)$$

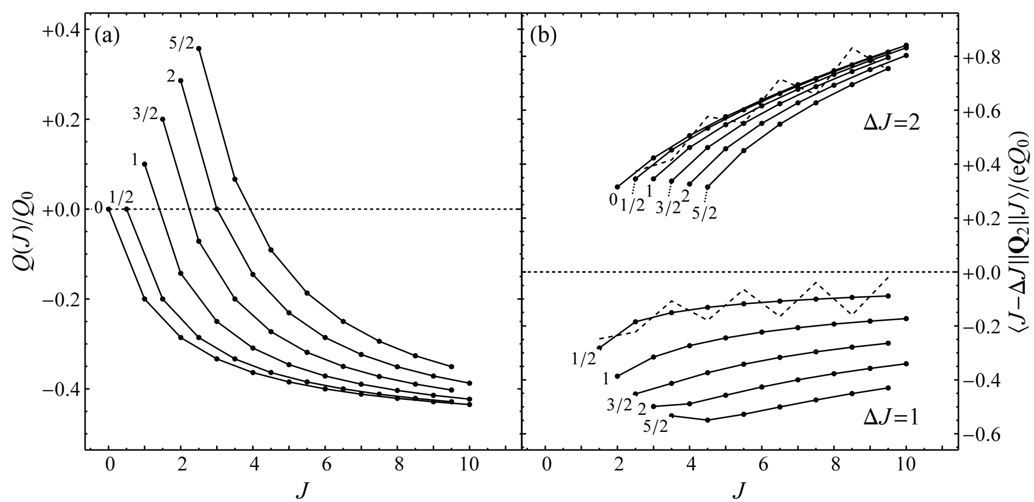
Rotational states: Quadrupole matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \frac{(2J_i+1)^{1/2}}{1+\delta_{K0}} \Big((J_i, K, 2, 0 | J_f, K) \langle \phi_K || E_{2,0} || \phi_K \rangle + (-)^{J_i+K} (J_i, -K, 2, 2K | J_f, K) \langle \phi_K || E_{2,2K} || \phi_{\bar{K}} \rangle \Big)$$

- Consider both proton and neutron quadrupole tensors
- Quadrupole moments

$$\mathcal{Q}(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} \mathcal{Q}_0$$

- Transition matrix elements



$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \sqrt{\frac{5}{16\pi}} \sqrt{2J_i+1} \, (J_i K 2 0 | J_f K) \, \mathcal{Q}_0$$

Rotational states: Dipole matrix elements

- Magnetic moments

$$\mu(J) = a_0\, J + a_1 \frac{K}{J+1} + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{2\sqrt{2}} \frac{2J+1}{J+1}$$

- Magnetic transition matrix elements

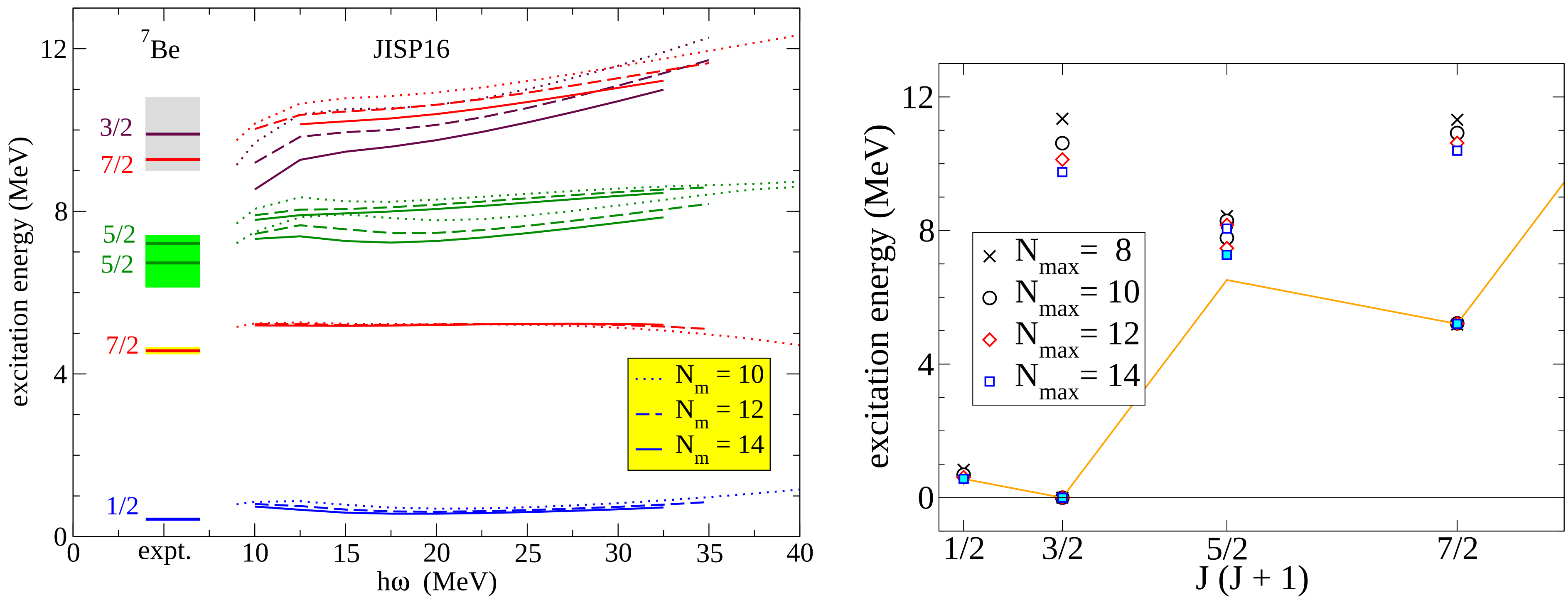
$$\langle \psi_{J-1,K} || M_1 || \psi_{J,K} \rangle = -\sqrt{\frac{3}{4\pi}} \sqrt{\frac{J^2 - K^2}{J}} \left(a_1 + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{\sqrt{2}} \right)$$

- Define dipole terms $D_{l,p}$, $D_{l,n}$, $D_{s,p}$, and $D_{s,n}$ for both the magnetic moments and for the M_1 transitions

$$M_1 = g_{l,p}\, D_{l,p} + g_{l,n}\, D_{l,n} + g_{s,p}\, D_{s,p} + g_{s,n}\, D_{s,n}$$

with $g_{l,p} = 1$, $g_{l,n} = 0$, $g_{s,p} = 5.586$, and $g_{s,n} = -3.826$

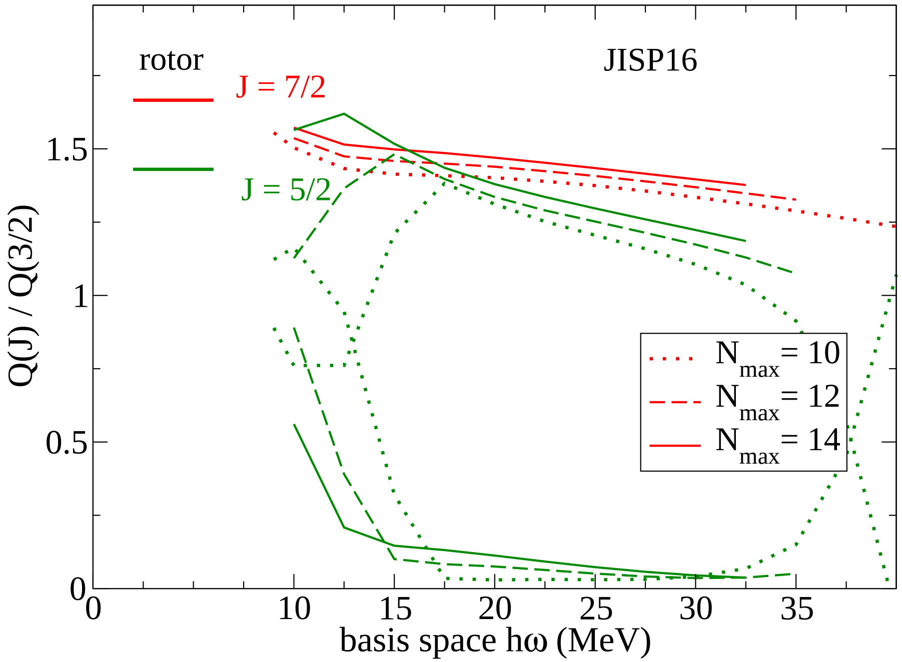
Excitation spectrum 7Be – Emergence of rotational band?

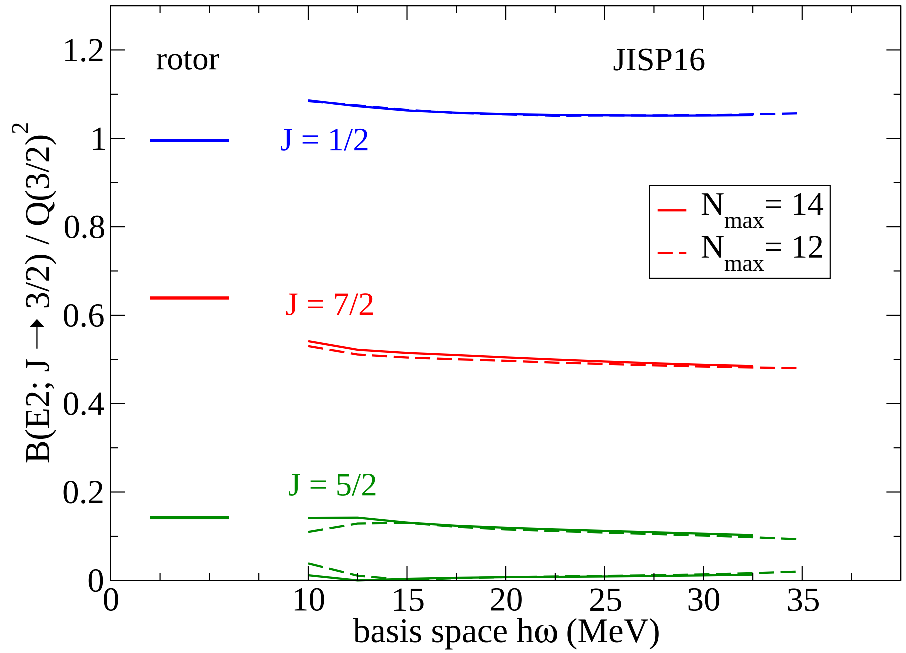


- Spectrum in reasonable agreement with data
  - lowest two excited states converged
  - broad resonances not as well converged
- Excitation energies of lowest J states consistent with $K = \frac{1}{2}$ rotational band

Emergence of $K = \frac{1}{2}$ rotational band

Ratio of electric quadrupole moments and B(E2)'s
over ground state quadrupole moment $\mathcal{Q}(3/2)$





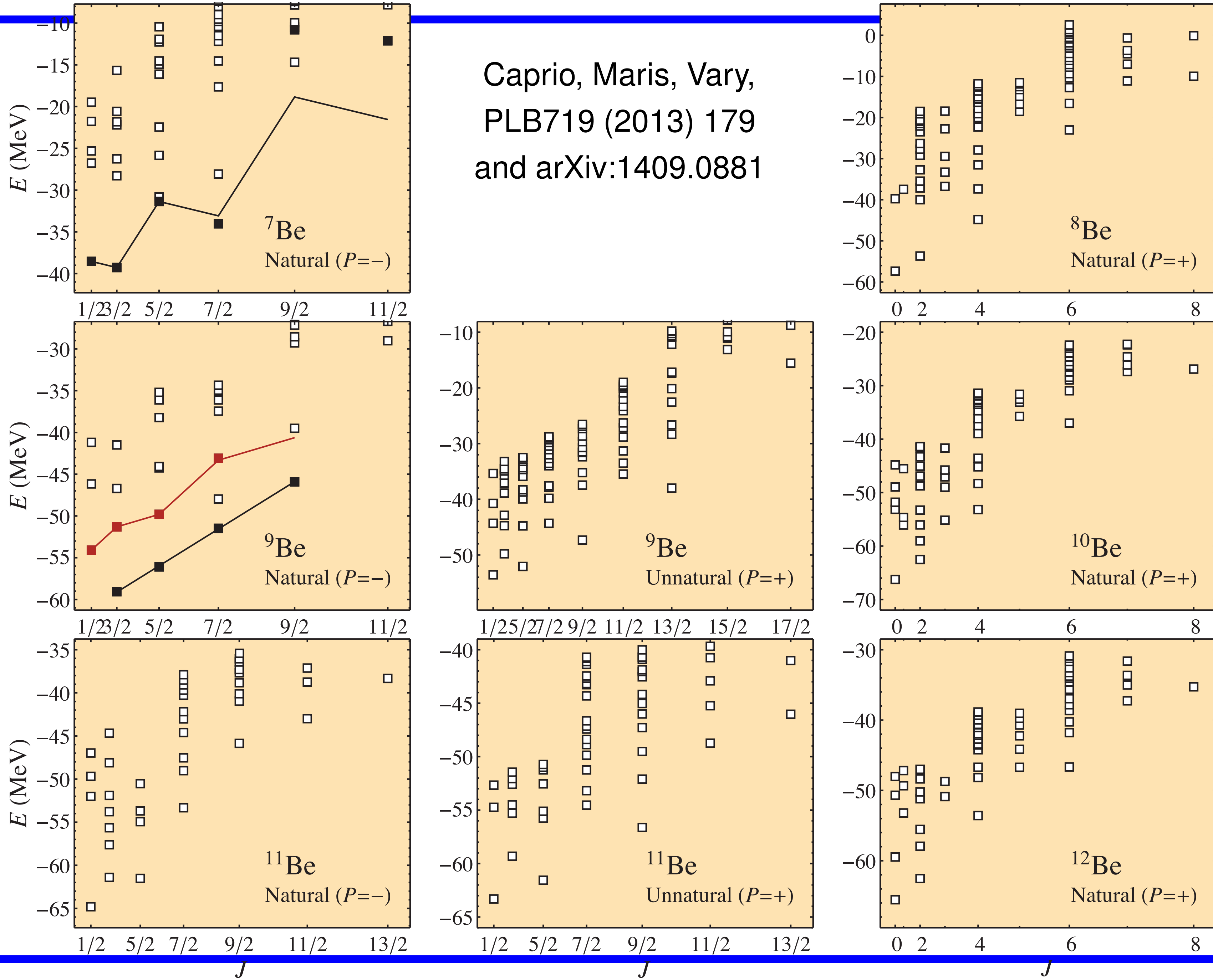
Rotor model

$$\mathcal{Q}(J) = \frac{\frac{3}{4} - J(J+1)}{(J+1)(2J+3)}\,\mathcal{Q}_0$$

$$B(E2; i \to f) = \frac{5}{16\pi}\left(J_i, \frac{1}{2}; 2, 0 \middle| J_f, \frac{1}{2}\right)^2 \mathcal{Q}_0^2$$

Candidate rotational bands: ^{7}Be–^{12}Be

Caprio, Maris, Vary,
PLB719 (2013) 179
and arXiv:1409.0881



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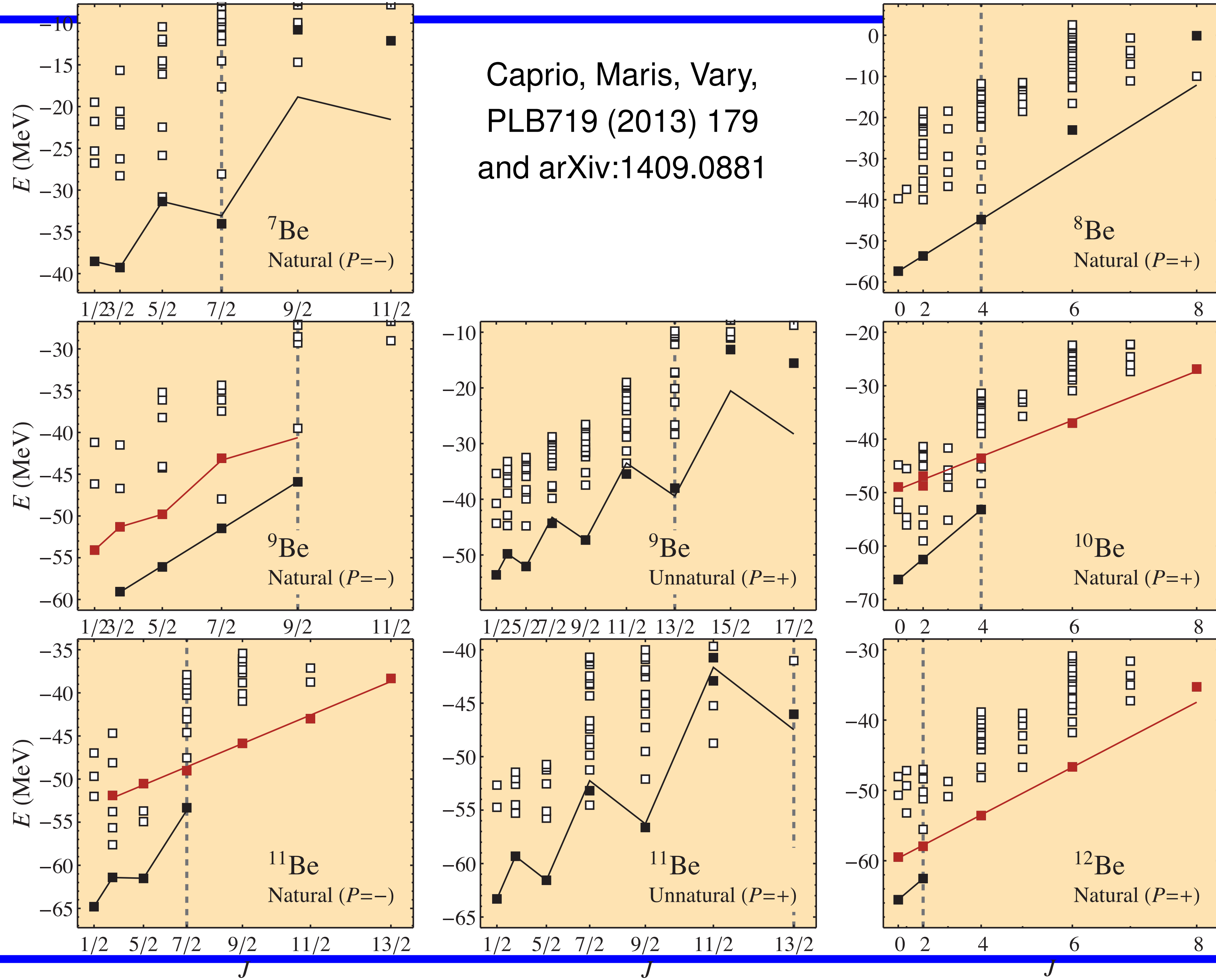
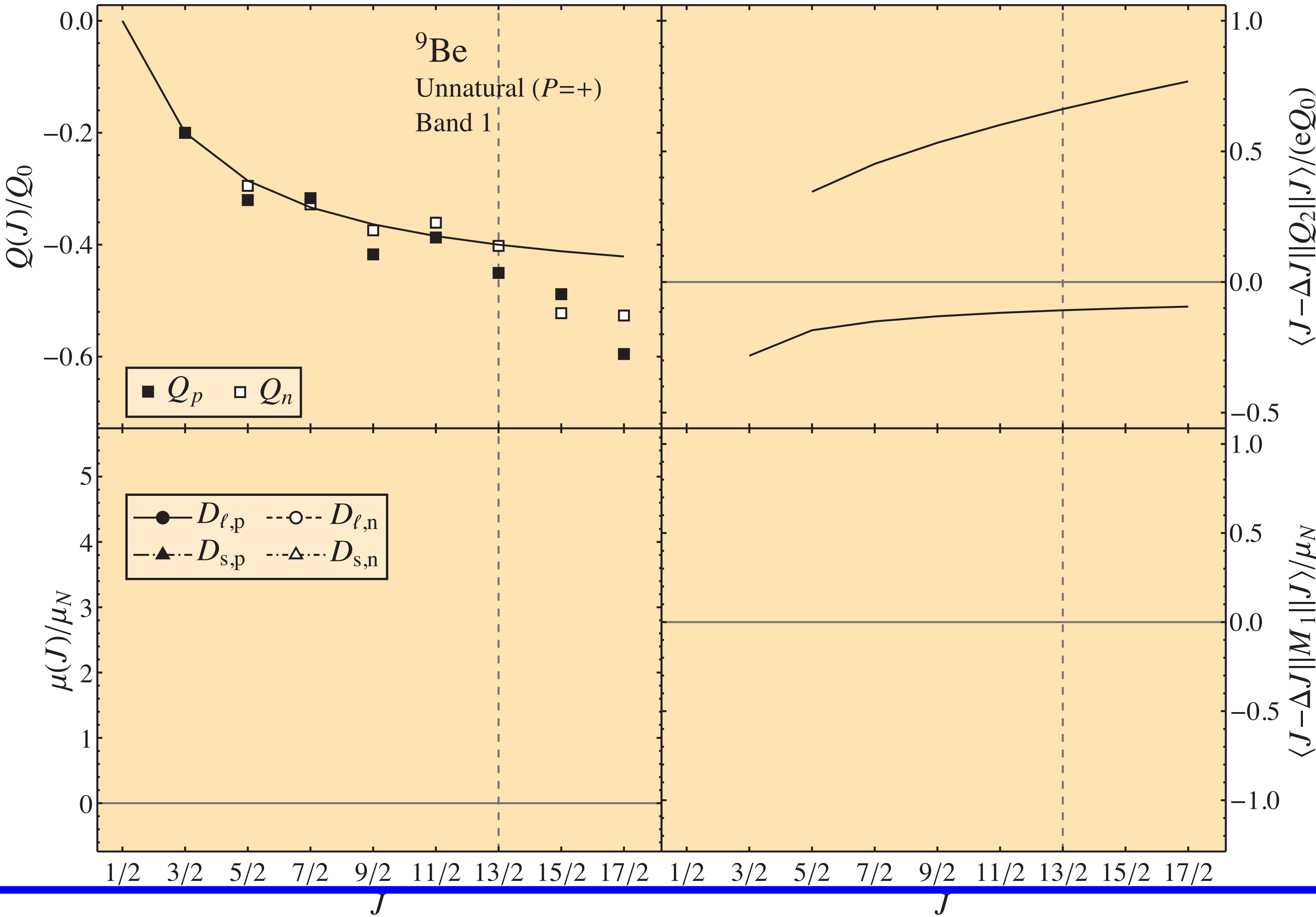
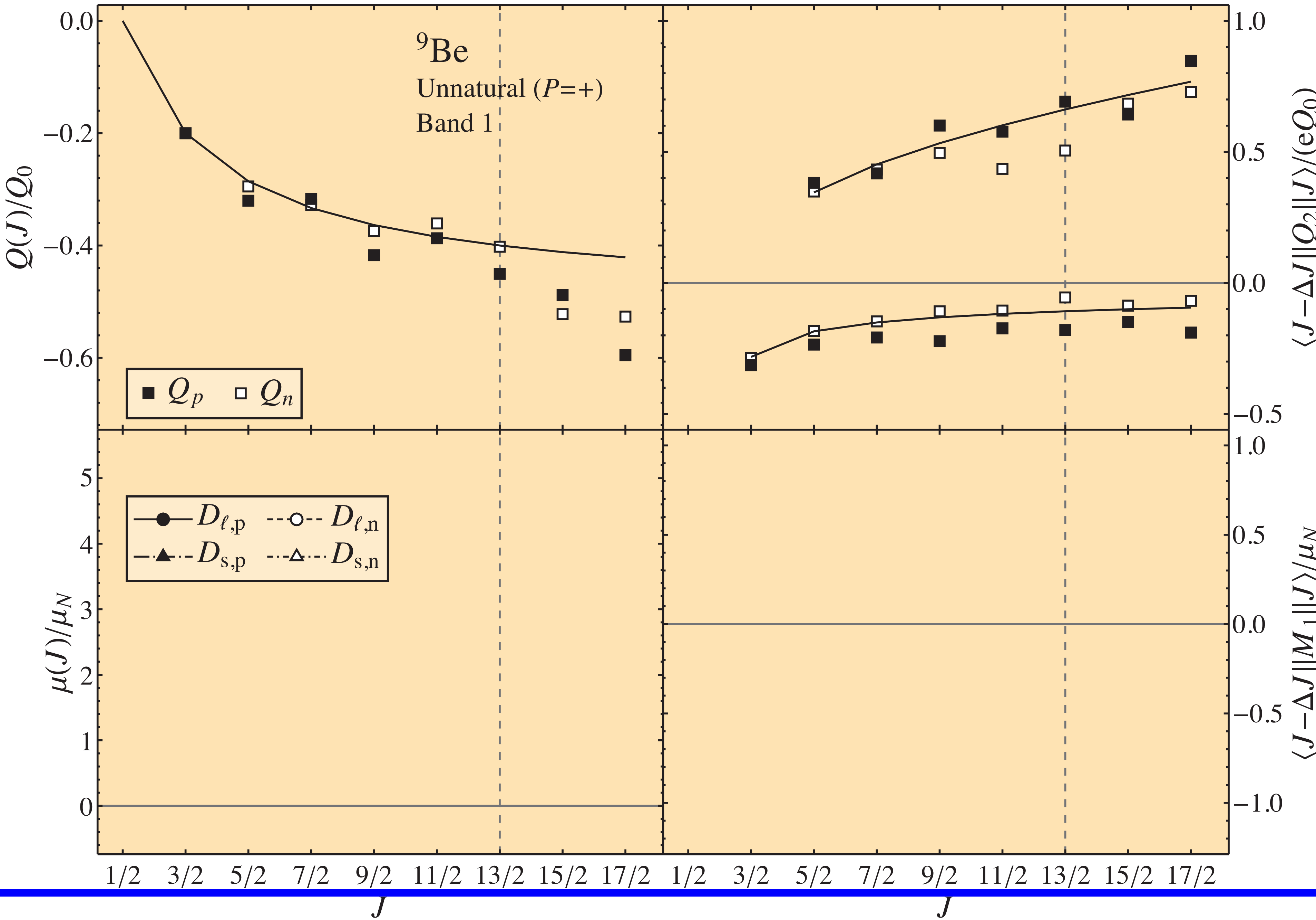


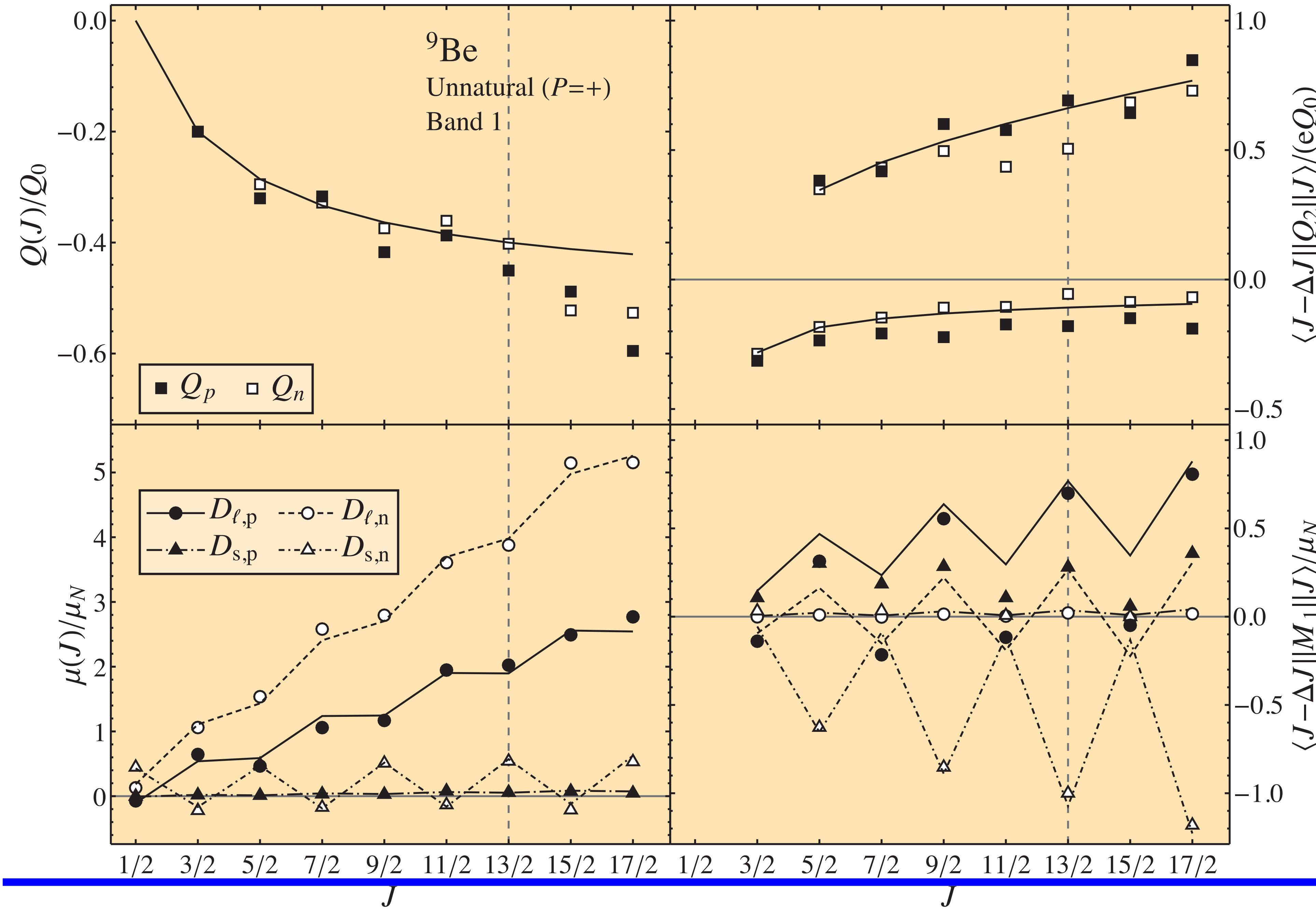
Electromagnetic moments and transitions



Electromagnetic moments and transitions



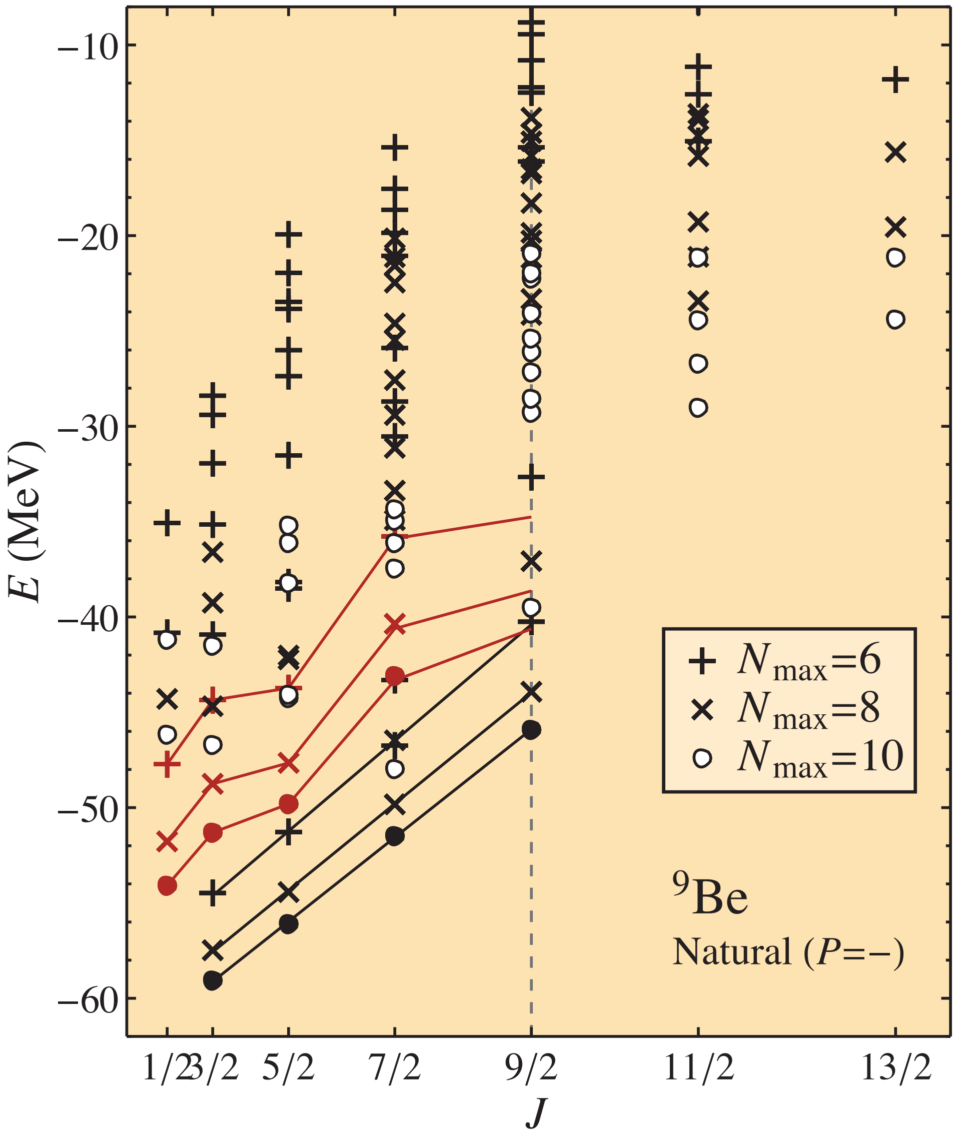
Electromagnetic moments and transitions

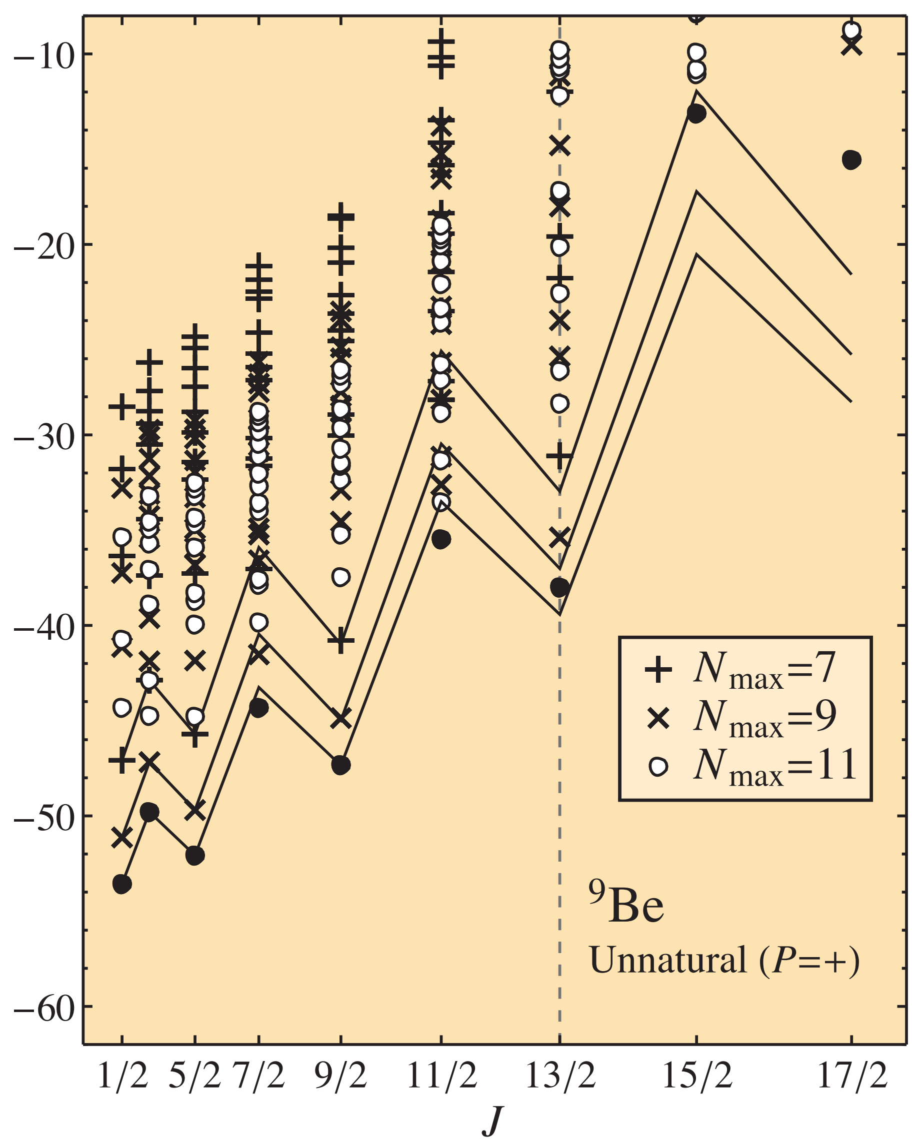


Convergence with basis size? ⁹Be

Absolute binding energy? **NO!**

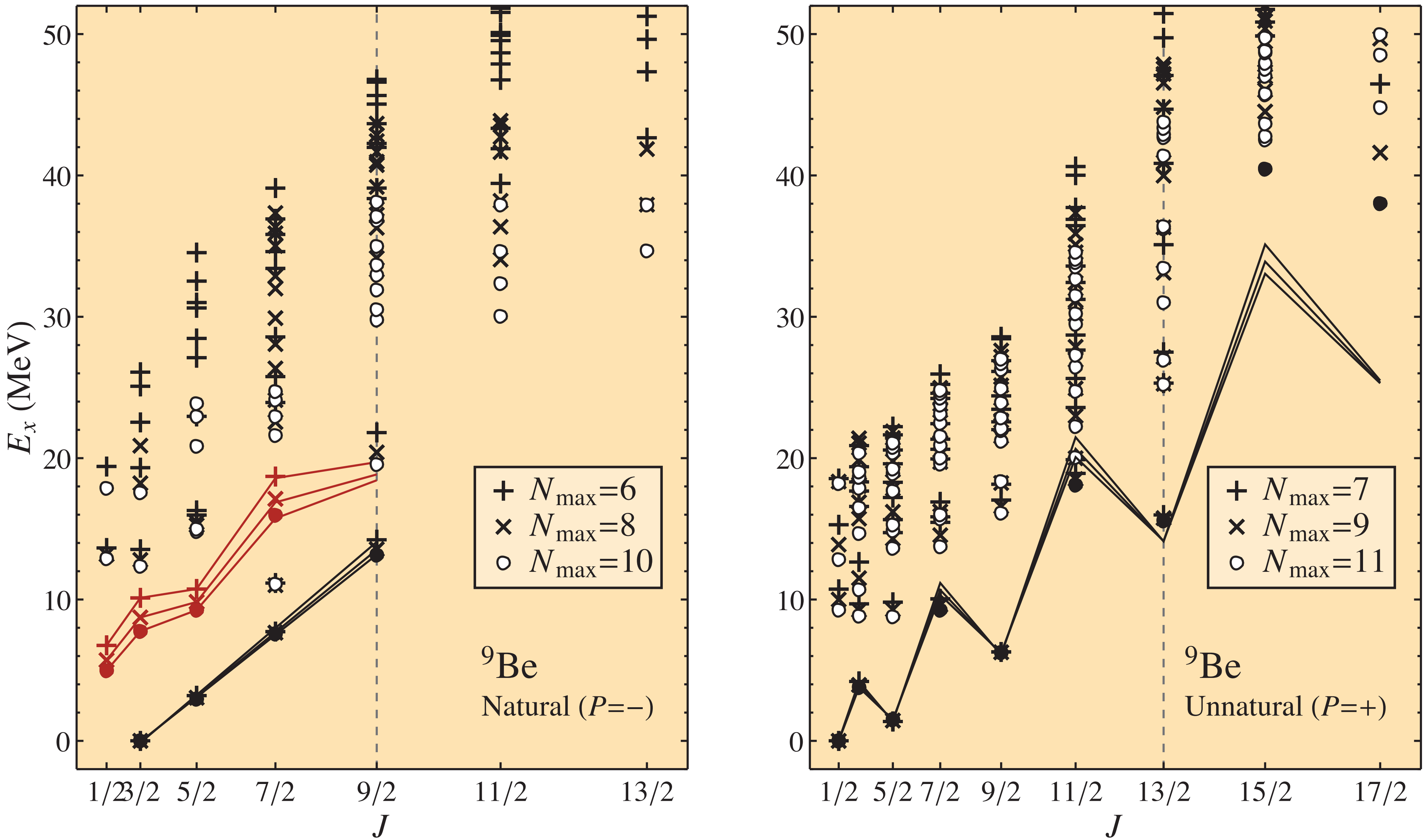
Maris, Caprio, Vary, arXiv:1409.0881





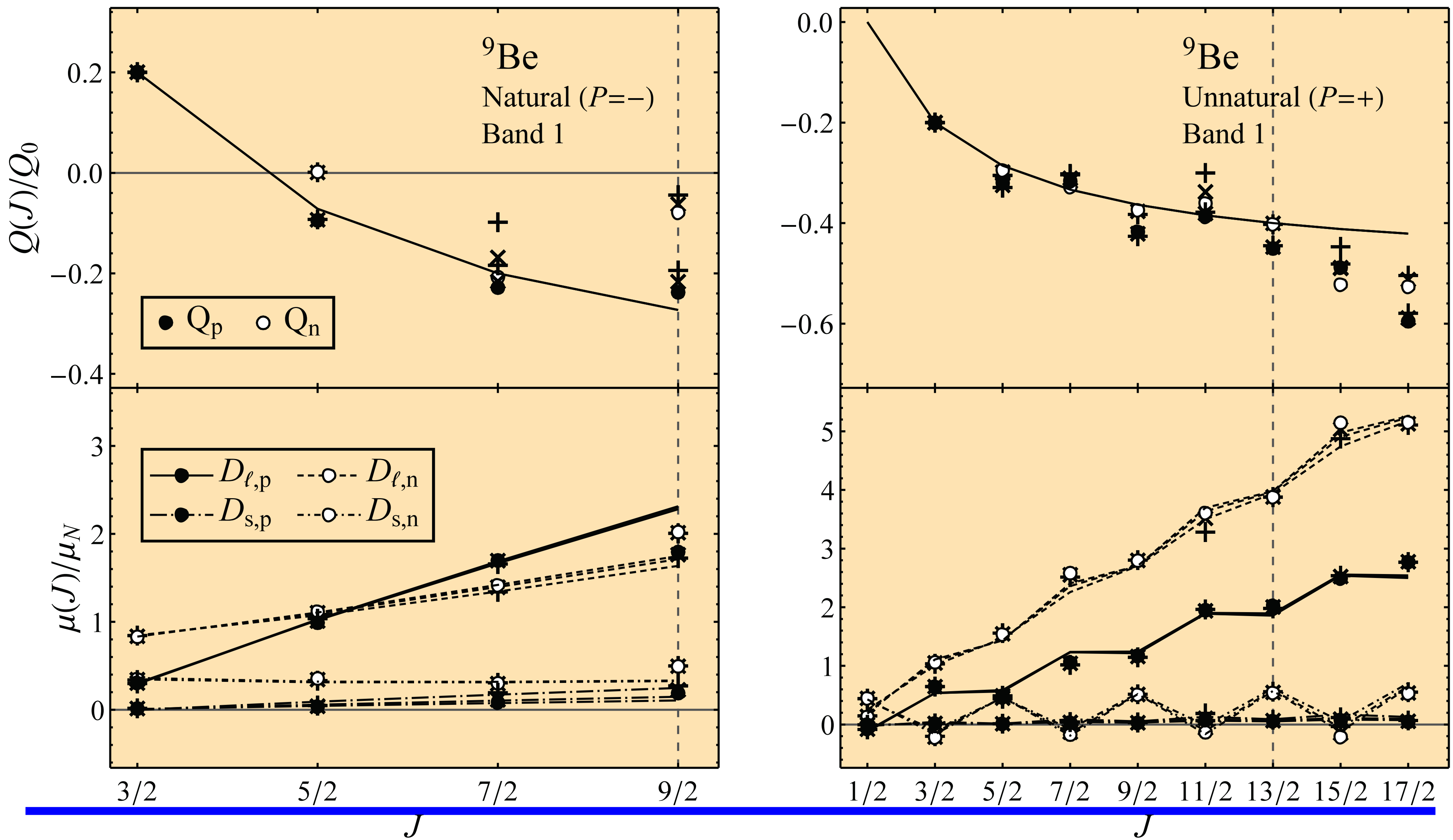
Convergence with basis size? ^{9}Be

Absolute binding energy? NO! Excitation within band? ~YES



Convergence with basis size? ^{9}Be

Absolute $E2$? **NO!** Ratio of $E2$? **~YES** Absolute $M1$? **~YES**



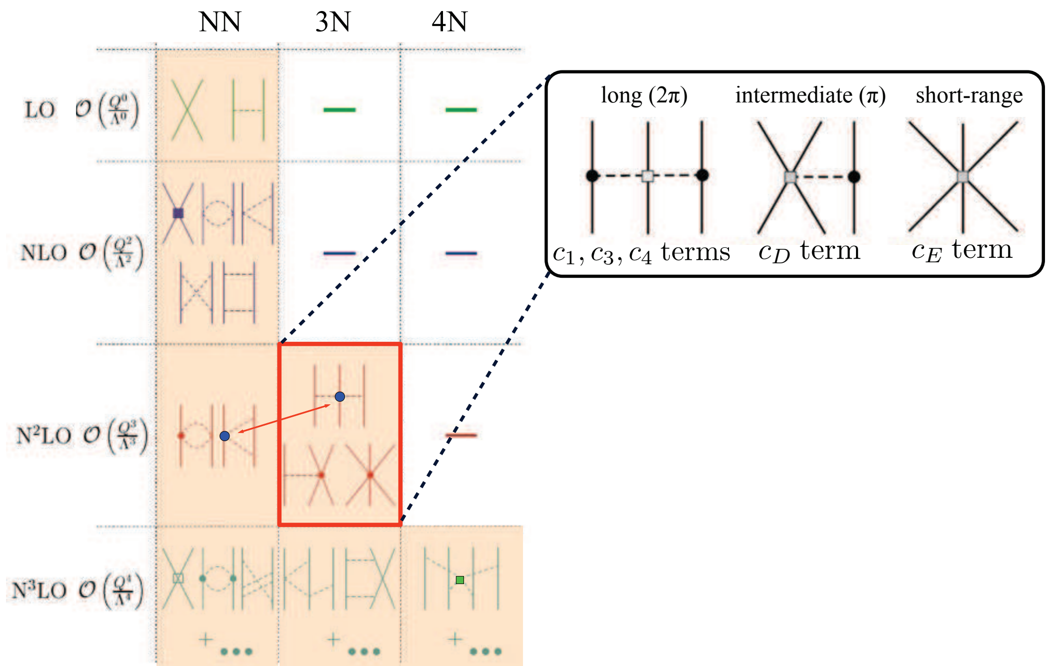
Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD   Entem and Machleidt, PRC68, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

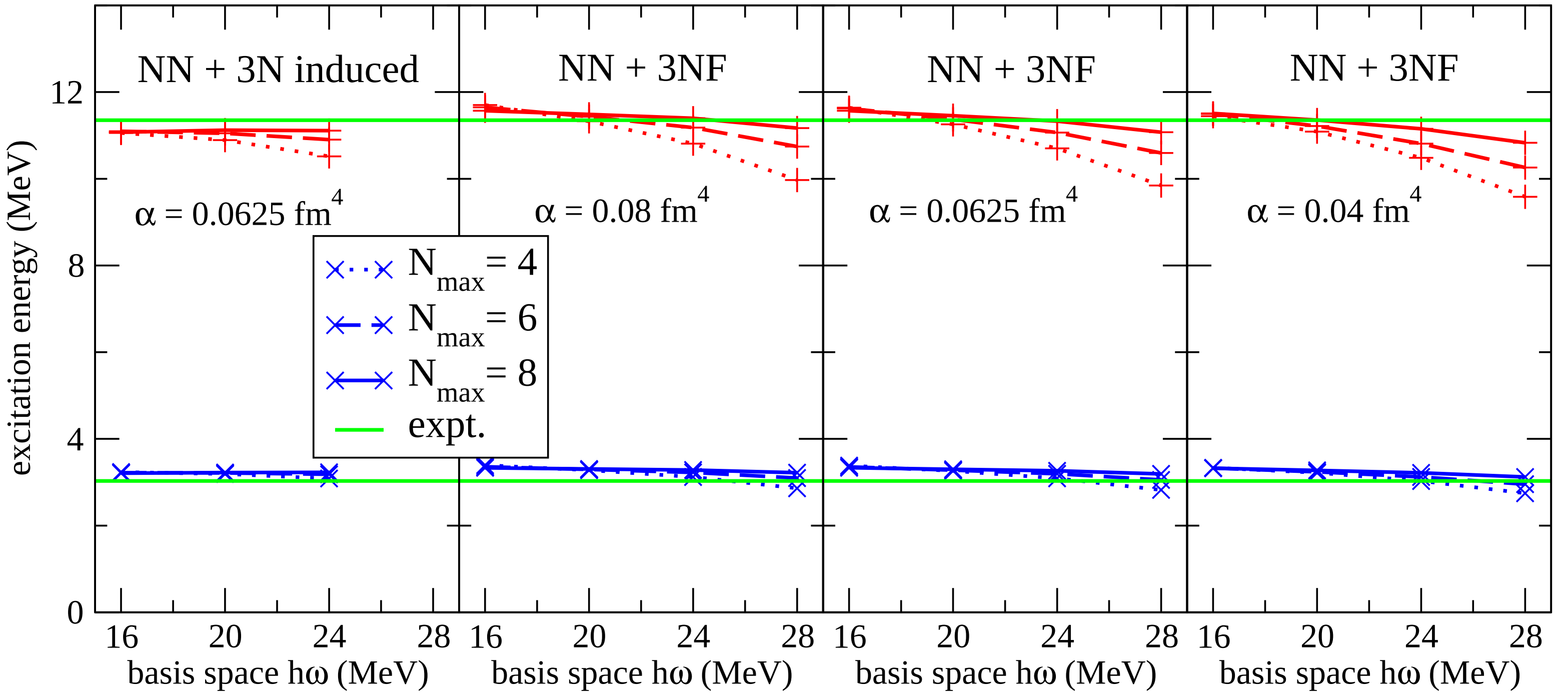
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



Effect of 3-body forces on rotational excited states ^{8}Be

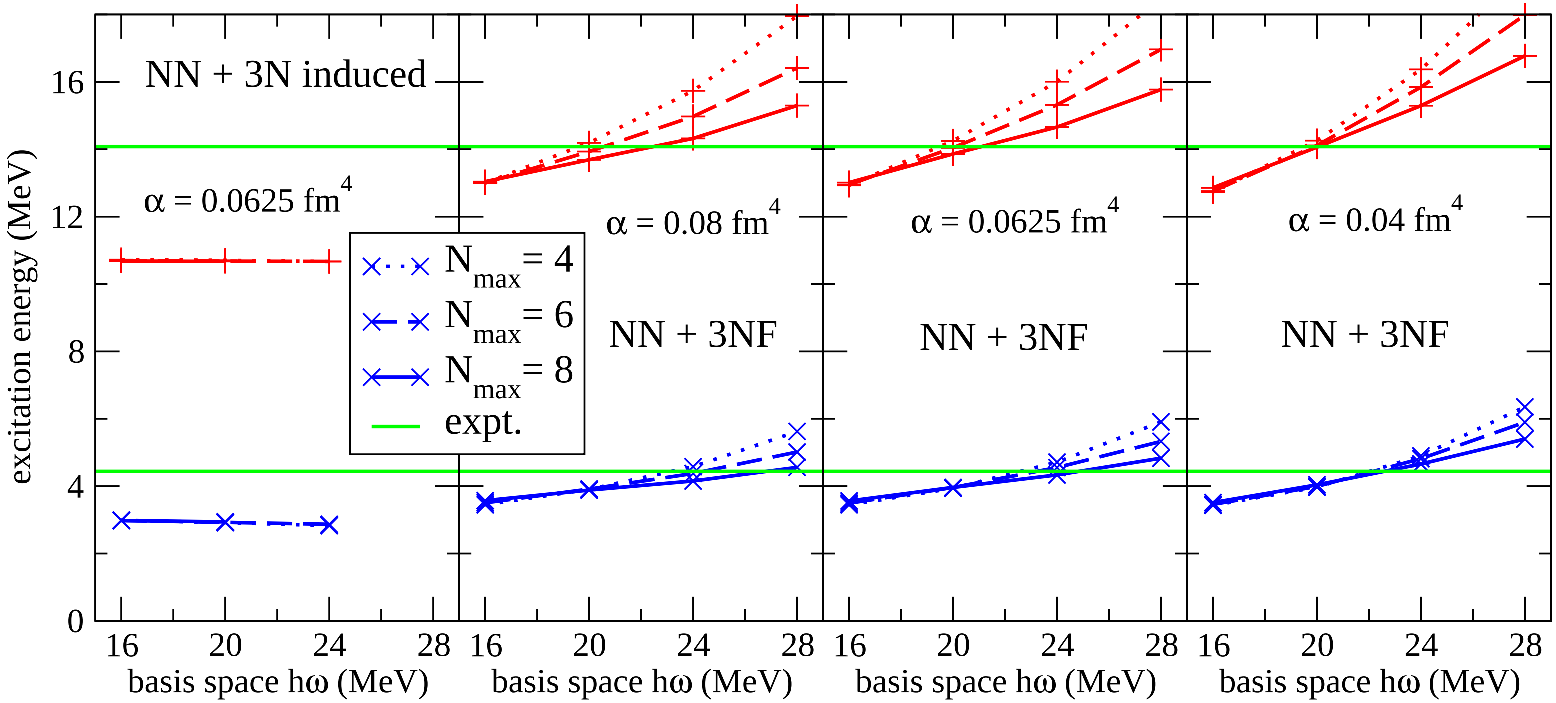
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)



- Qualitative agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Ratio's of excitation energies, quadrupole moments and B(E2)'s in agreement with rotational model

Effect of 3-body forces on rotational excited states ^{12}C

Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)



- Chiral 3NF improves agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Increase in excitation energy of $(2^+, 0)$ and $(4^+, 0)$ rotational states likely due to increased binding of $(0^+, 0)$

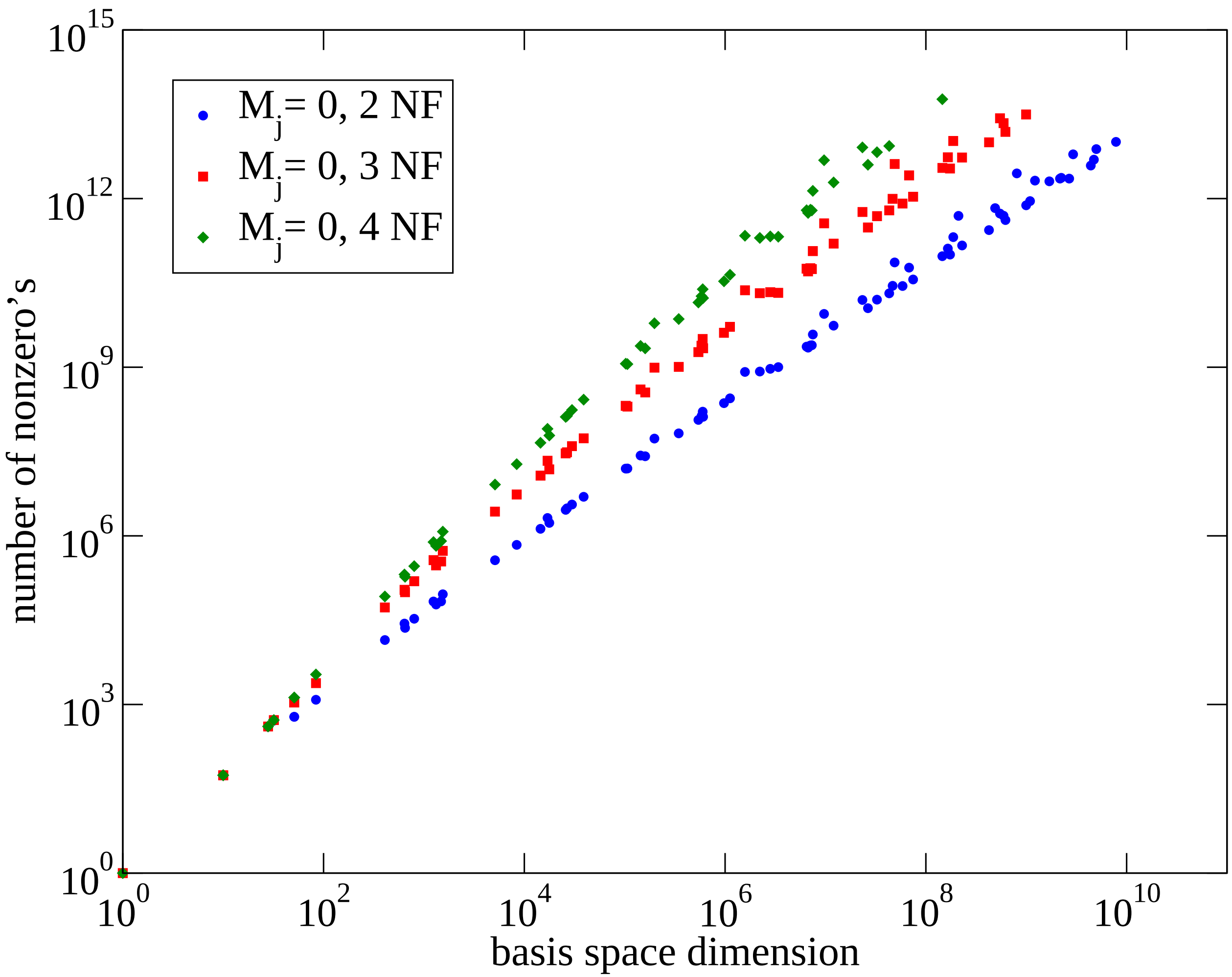
Conclusions

- No-core Configuration Interaction nuclear structure calculations
  - Main challenge: construction and diagonalization of extremely large (D $\sim 10^{10}$) sparse (NNZ $\sim 10^{14}$) matrices
- Emergence of rotational structure
  - Excitation energies (i.e. energy differences)
  - Ratios of Q moments and E2 transition matrix elements
  - Dipole moments and M1 transition matrix elements
- Perspectives
  - Convergence of long-range observables remains a challenge
    - extrapolation tools
    - efficient truncation schemes w. uncertainty estimates
    - realistic basis functions w. correct asymptotic behavior
  - Resonance state: incorporating continuum

  NESAP award – early science project on Cori NERSC (Xeon Phi)
- Would not have been possible without collaboration with applied mathematicians and computer scientists

Looking forward: Taming the scale explosion

- Reaching the limit of M-scheme N_{max} truncation
  - extremely large, extremely sparse matrices

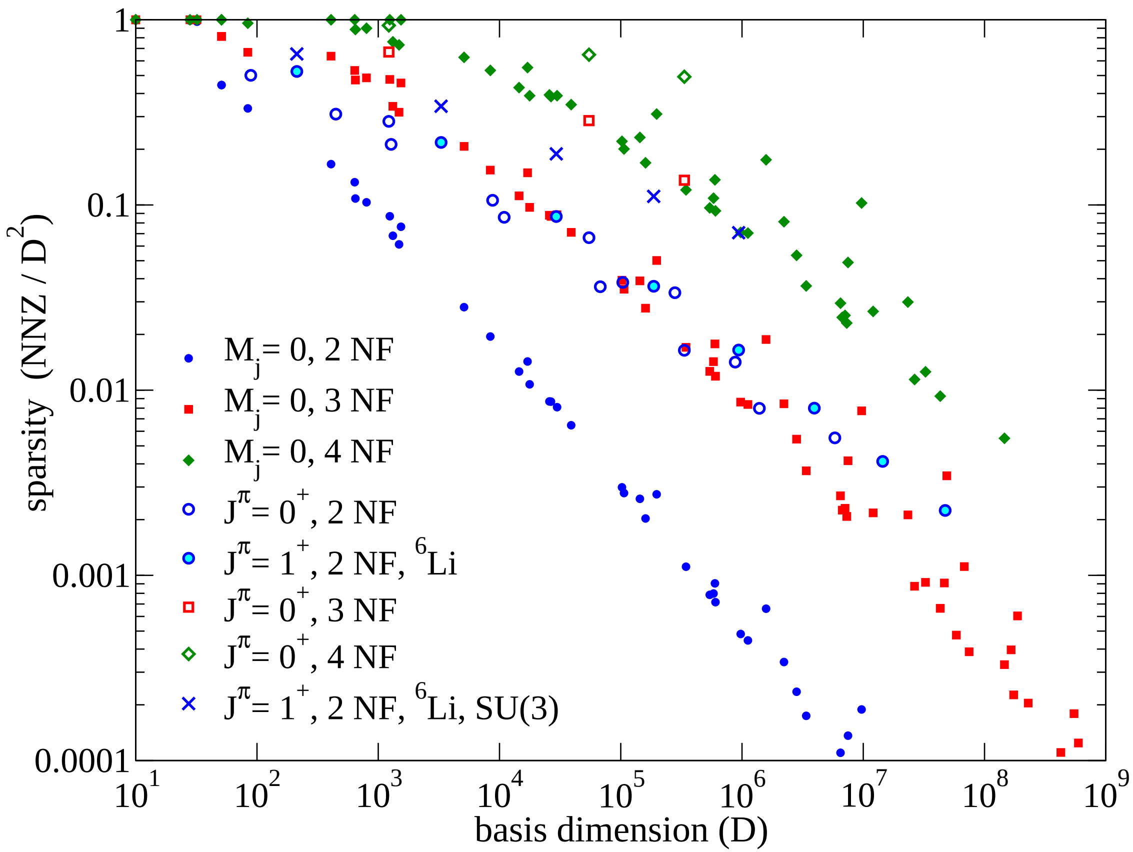


number of nonzero's in M-scheme, $M_j = 0$ for $N = Z$ nuclei from ^{6}Li to ^{20}Ne

- Hopper: 212 TB
  $26 \cdot 10^{12}$
- Edison: 333 TB
  $41 \cdot 10^{12}$
- Titan: 600 TB (CPUs)
  $75 \cdot 10^{12}$
- Mira: 768 TB
  $95 \cdot 10^{12}$
- Blue Waters: 1.4 PB
  $170 \cdot 10^{12}$

Looking forward: *Taming the scale explosion*

- Reaching the limit of M-scheme N_{max} truncation
- Exploit symmetries to reduce basis dimension
  - Coupled-J basis — Aktulga, Yang, Ng, Maris, Vary, HPCS2011
  - SU(3) basis — Dytrych *et al*, PRL111, 252501 (2013)

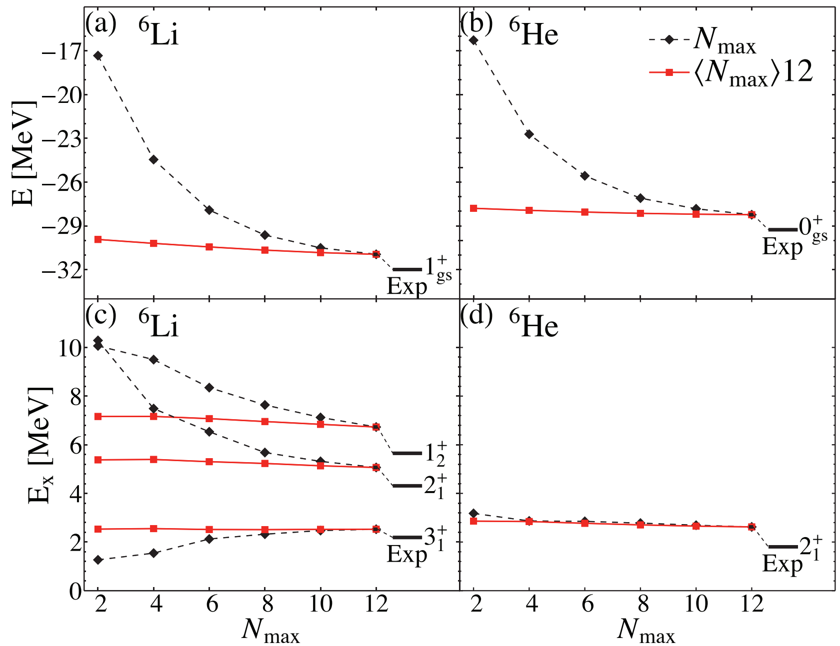


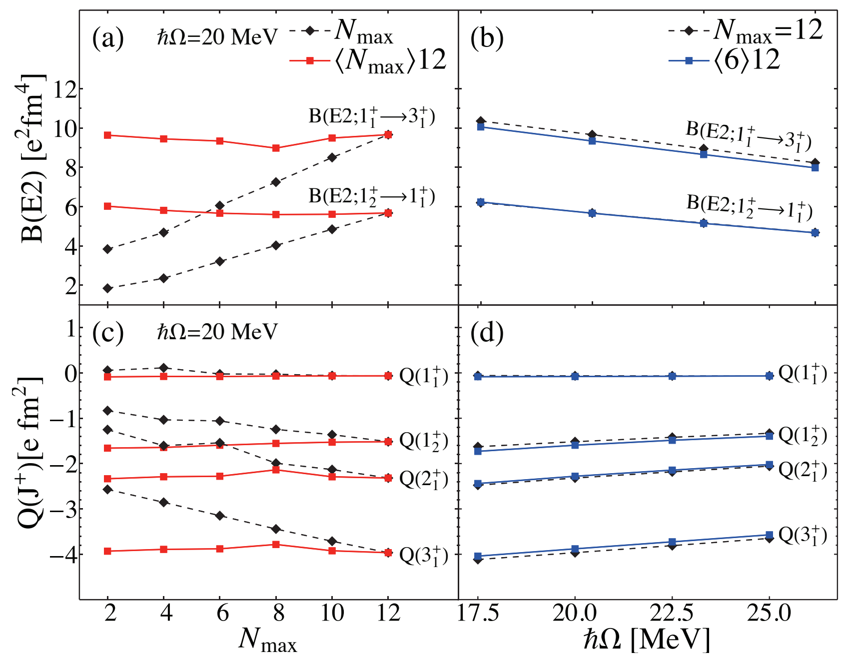
- smaller, but less sparse matrices
- number of nonzero matrix elements often (significantly) larger than in M-scheme
- construction of matrix more costly
- larger memory footprint than in M-scheme

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

Dytrych *et al*, PRL111, 252501 (2013)





- $\langle N_{\max}\rangle 12$ complete basis up to $N_{\max}$, dominant SU(3) irreps up to $N_{\max} = 12$
- Exact factorization (in combination with HO s.p. basis)
- Calculations for ^{12}C and ^{20}Ne in progress

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

  Dytrych *et al*, PRL111, 252501 (2013)

- No-Core Monte-Carlo Shell Model

  Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)

  - based on FCI truncation, not on N_{max} truncation
  - reduce basis to (few) hundred highly optimized states
  - coupled-J basis
  - leads to small but dense matrix

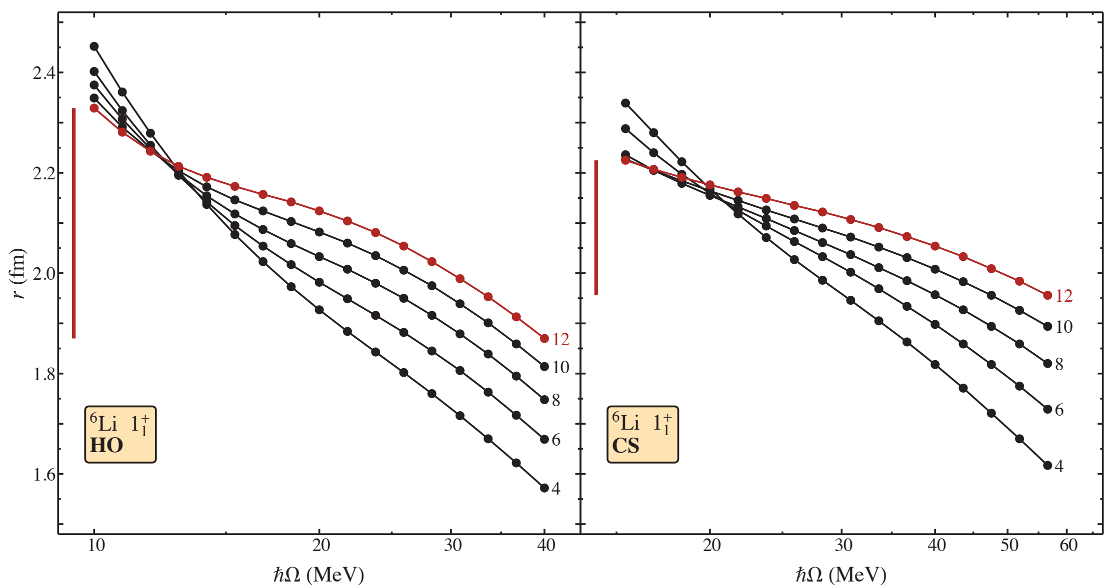
- Importance Truncated NCSM — Roth, PRC79, 064324 (2009)
  - based on N_{max} truncation
  - reduce basis dimension by (several) order(s) of magnitude
  - many-body states single Slater Determinants in M-scheme

Caveat: Uncertainty Quantification

- Can the numerical errors due to reduced basis dimension be quantified within the computation framework?

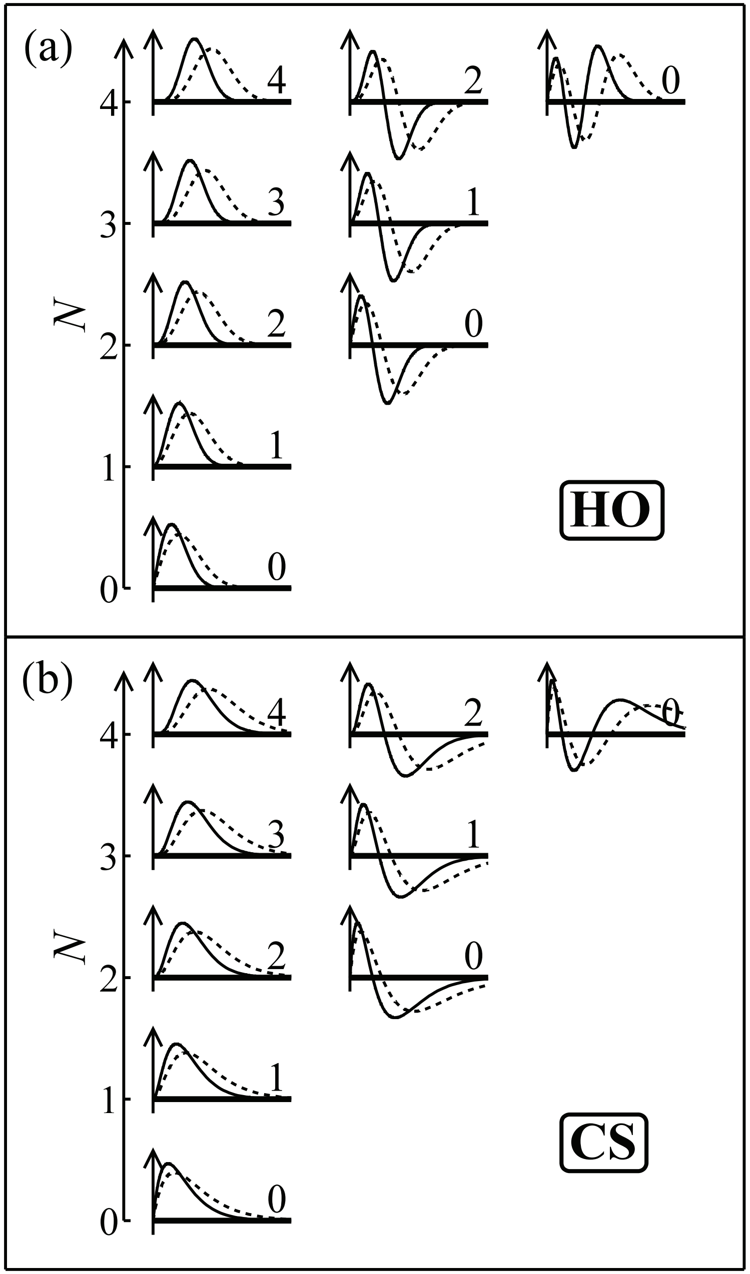
Beyond Harmonic Oscillator wavefunctions

- Berggren basis / No-Core Gamow Shell Model
  - incorporate continuum into basis
  - diagonalize complex symmetrix matrix
- Coulomb–Sturmian basis
  - radial basis functions with exponential asymptotic behavior



e.g. Coulomb–Sturmian basis to improve convergence of RMS radius, Caprio, Maris, Vary, PRC86, 034312 (2012)

Coulomb–Sturmian basis



Caprio, Maris, Vary, PRC86, 034312 (2012);
PRCC90, 034305 (2014)

- Harmonic Oscillator radial w.f.

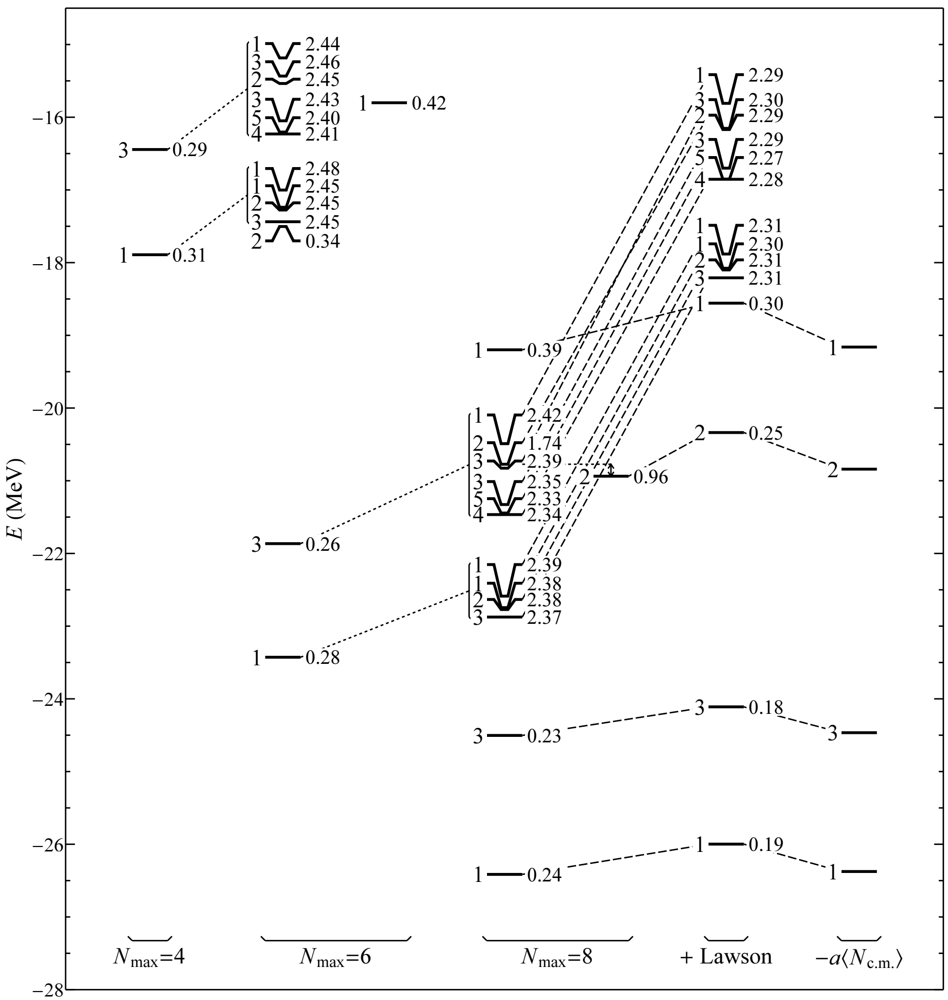
$$R_{nl}(b;r) = \left(\frac{r}{b}\right)^{l+1} L_n^{l+\frac{1}{2}}\left((r/b)^2\right) e^{-\frac{1}{2}(r/b)^2}$$

- Coulomb–Sturmian radial w.f.

$$S_{nl}(b;r) = \left(\frac{2r}{b}\right)^{l+1} L_n^{2l+2}(2r/b)\, e^{-r/b}$$

- Length scale b_l choosen such that nodes of $n = 1$ CS and HO w.f. coincide
- CS basis
  - truncation on $\sum(2n+l)$ for comparison with HO basis
  - no exact factorization of CM motion

Center-of-Mass motion

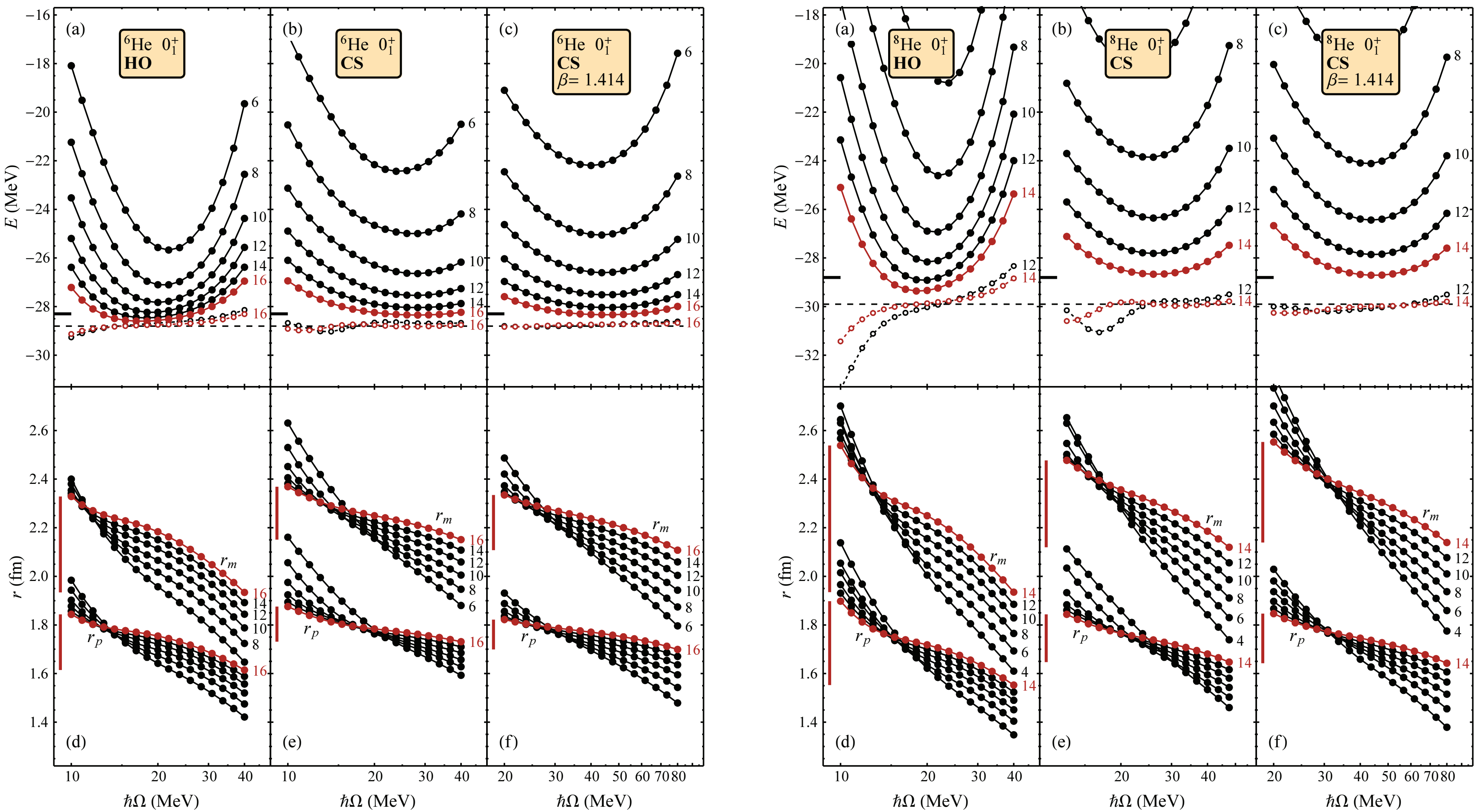


Caprio, Maris, Vary,
PRC86, 034312 (2012)

- Without Lagrange multiplier
  - at $N_{\text{max}} = 6$
    - 4 degenerate states: $J^\pi = 1^+$ states at $N_{\text{max}} = 4$ with 2 quanta CM excitations
    - 6 degenerate states: $J^\pi = 3^+$ states at $N_{\text{max}} = 4$ with 2 quanta CM excitations
  - degenerate states at $N_{\text{max}} = 8$:
    - 1^+ and 3^+ states at $N_{\text{max}} = 6$ with 2 quanta CM excitations
    - 1^+ and 3^+ states at $N_{\text{max}} = 4$ with 4 quanta CM excitations
- With Lagrange multiplier all states with CM excitations are removed from low-lying spectrum

Coulomb–Sturmian for halo nuclei

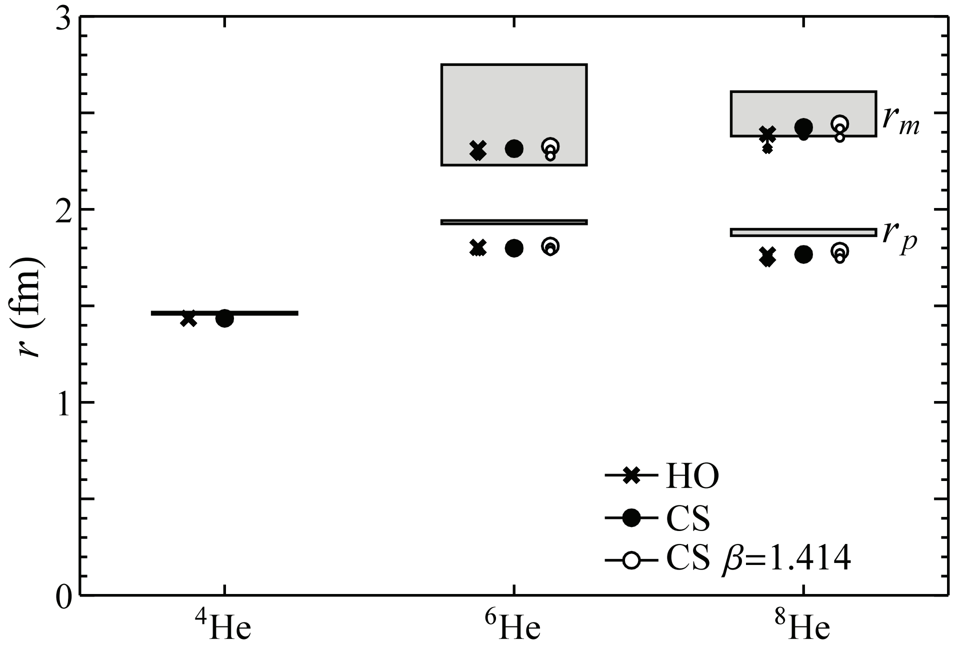
Caprio, Maris, Vary, PRC90, 034305 (2014)



- CS: different length parameters b_l for protons and neutrons

Radii of He isotopes with JISP16

Caprio, Maris, Vary, PRC90, 034305 (2014)



- Radii exctracted from crossover point for three highest $N_{\max}$ values
- HO and CS basis in good agreement with each other
- Qualitative agreement with data
- Note: matter radii in agreement with elastic scattering measurement/extraction of experimental radius

Future plans

- Explore different basis truncation schemes
- Apply to chiral NN and 3N interactions